

# Coupled-cluster calculations for valence systems around $^{16}\text{O}$

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We study the ground and low-lying excited states of  $^{15}\text{O}$ ,  $^{17}\text{O}$ ,  $^{15}\text{N}$ , and  $^{17}\text{F}$  using modern two-body nucleon-nucleon interactions and the suitably designed variants of the *ab initio* equation-of-motion coupled-cluster theory aimed at an accurate description of systems with valence particles and holes. A number of properties of  $^{15}\text{O}$ ,  $^{17}\text{O}$ ,  $^{15}\text{N}$ , and  $^{17}\text{F}$ , including ways the energies of ground and excited states of valence systems around  $^{16}\text{O}$  change as functions of the number of nucleons, are correctly reproduced by the equation-of-motion coupled-cluster calculations. Within a harmonic oscillator basis and large effective model spaces, our results are converged for the chosen two-body Hamiltonians. Thus, all disagreements with experiment are, most likely, due to the degrees of freedom such as three-body interactions not accounted for in our effective two-body Hamiltonians. In particular, the calculated binding energies of  $^{15}\text{O}/^{15}\text{N}$  and  $^{17}\text{O}/^{17}\text{F}$  enable us to rationalize the discrepancy between the experimental and recently published [Phys. Rev. Lett. **94**, 212501 (2005)] equation-of-motion coupled-cluster excitation energies for the  $J^\pi = 3^-$  state of  $^{16}\text{O}$ . The results demonstrate the feasibility of the equation-of-motion coupled-cluster methods to deal with valence systems around closed-shell nuclei and to provide precise results for systems beyond  $A = 16$ .

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## I. INTRODUCTION

The way shell closures and single-particle energies evolve as functions of the number of nucleons is presently one of the greatest challenges to our understanding of the basic features of nuclei. The properties of single-particle energies and states with a strong quasi-particle content along an isotopic chain are moreover expected to be strongly influenced by the nuclear spin-orbit force. The latter can be retraced to contributions from both two-body and three-body models of the nuclear forces (see, for example, Refs. [1, 2]). A fully microscopic *ab initio* description of masses, shell closures, excited states, and single-particle energies in terms of the underlying nuclear forces is an unresolved problem in nuclear physics that awaits a satisfactory and computationally tractable solution.

For light nuclei with mass numbers  $A \leq 12$ , both Green's function Monte Carlo methods [3] and large-scale no-core shell-model calculations [4] provide almost converged benchmarks for selected two- and three-body Hamiltonians, where typically the models for the two-body nucleon-nucleon interactions reproduce the available scattering data, while the three-body interaction models are normally fitted to reproduce the binding energies of selected nuclei. The agreement with experimental data for many light nuclei is in these calculations quite reasonable. Unfortunately, for medium-mass and heavier nuclei the dimensionality of the corresponding many-particle problem becomes intractable by the Green's function Monte Carlo methods and *ab initio* no-core shell-model techniques, and one typically has to

resort to a simplified shell-model description within a smaller space, the so-called model space. In order to solve the corresponding many-body Schrödinger equation, one needs then to derive effective two and/or three-body interactions for the chosen small model space. Many-body perturbation theory is normally employed to derive effective interactions [5], but unless these interactions are fitted to reproduce selected properties of nuclei [6, 7], one cannot correctly recover the experimentally derived single-particle and excitation energies and shell closures (see, for example, Ref. [8]).

Two key points make it imperative to investigate new theoretical methods that will allow for an accurate description of closed- as well as open-shell nuclei with  $A \gg 12$ . First, present and proposed nuclear structure research facilities will open significant territory into regions of medium-mass and heavier nuclei, where the majority of the studied nuclei will be open-shell systems and where many of the nuclei produced in experiment will be unstable or short-lived. Second, existing shell-model and Green's function Monte Carlo techniques have prohibitive computer costs that scale factorially or exponentially with the system size. In addition to an increased dimensionality, one needs to account for the fact that many of the medium-mass and heavier nuclei can be weakly bound and couple to resonant states. Moreover, in order to examine new nuclei that have not been discovered or studied before, one may not be able to rely on fitting the effective Hamiltonians to the experimental data for the known nuclei, as has been traditionally done for many years. Microscopic *ab initio* methods, in which nuclear properties are obtained from the underlying nucleon-nucleon interactions, will become in-

creasingly important as the new information about the medium-mass and heavier nuclei is obtained in various experiments. In addition to these practical aspects, *ab initio* calculations of nuclear properties, including, for example, the way the binding and excitation energies change as a function of the number of nucleons around closed-shell nuclei, may provide important new insights into our understanding of nuclear forces.

Clearly, if we wish to extend *ab initio* methods to nuclei with  $A \gg 12$ , we have to consider alternatives to the existing Green's function Monte Carlo and no-core shell-model techniques. In this work, we focus on coupled-cluster theory [9, 10, 11, 12], which is a promising candidate for the development of practical methods for fully microscopic *ab initio* studies of nuclei in the  $A \gg 12$  mass region. As has been demonstrated over and over again in numerous quantum chemistry applications (see, e.g., Refs. [13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23] for selected reviews), coupled-cluster methods are capable of providing a precise description of many-particle correlation effects at the relatively low computer costs, when compared to shell-model or configuration interaction techniques aimed at similar accuracies. Based on the remarkable success of coupled-cluster methods in chemistry and molecular physics, where one has to obtain a highly accurate description of many-electron correlation effects, we believe that the field of nuclear physics may significantly benefit from the vast experience in the development of accurate and computationally efficient coupled-cluster approximations and algorithms by quantum chemists.

Although historically coupled-cluster theory originated in nuclear physics [9, 10], its applications to the nuclear many-body problem have been relatively rare (see, e.g., Refs. [24, 25, 26], and references therein), particularly when compared to quantum chemistry. For many years, part of the problem has been an inadequate understanding of nucleon-nucleon interactions and lack of adequate computer resources in the 1970s and 1980s. This situation has changed only in the last few years. The successful construction of realistic nucleon-nucleon potentials (cf., e.g., Refs. [27, 28, 29, 30]) and spectacular improvements in computer technology have led to renewed interest in applying coupled-cluster methods in *ab initio* nuclear physics calculations. In particular, using bare interactions, Mihaila and Heisenberg performed impressive coupled-cluster calculations for the binding energy and the electron scattering form factor of  $^{16}\text{O}$  [31, 32, 33, 34]. We have taken an alternative route and combined a few basic coupled-cluster techniques, developed earlier in the context of electronic structure studies by quantum chemists, with the renormalized form of the Hamiltonian to determine ground and selected excited states of  $^4\text{He}$  and  $^{16}\text{O}$  [35, 36, 37, 38, 39, 40], demonstrating promising results when compared with the results of the exact shell-model diagonalization in the same model space [36] and, at least for some properties, with the experimental data [35, 37, 38, 39, 40]. In particular, in our most recent study of the ground and excited states of

$^{16}\text{O}$  [37], we obtained fully converged results which are very close to those obtained with more expensive large-scale no-core shell-model calculations of Navrátil and collaborators [41]. This has been possible thanks to the use of the elegant diagram factorization techniques developed by quantum chemists [42], which lead to almost perfectly vectorized [23, 43, 44] and highly scalable parallel [35] computer codes, enabling routine calculations for systems in the  $A \sim 20$  region with large single-particle basis sets, including seven or even eight major oscillator shells (336 and 480 single-particle states, respectively). It should be emphasized that although we are still in the early stages of developing a library of efficient, general-purpose coupled-cluster programs for nuclear structure applications, there are already several differences between our approach to nuclear coupled-cluster calculations and the approach pursued by Mihaila and Heisenberg [31, 32, 33, 34]. First of all, Mihaila and Heisenberg used bare interactions, making the convergence with the number of single-particle basis states very slow, whereas we use the renormalized form of the Hamiltonian exploiting, for example, a no-core G-matrix theory [35], which leads to a rapid convergence of binding and excitation energies and other nuclear properties with the number of major oscillator shells in a basis set [35, 37, 38, 39, 40]. Second, we are able to calculate ground as well as excited states, not just the ground-state properties of closed-shell nuclei examined by Mihaila and Heisenberg. Finally, as mentioned above, our coupled-cluster computer codes have been developed using diagram factorization techniques, which minimize the CPU operation count, rather than the commutator expansions used by Mihaila and Heisenberg and the Bochum school. The coding style adopted by us is similar to that practiced by the lead developers of coupled-cluster methods in chemistry. In particular, we put an emphasis on the general-purpose character of our codes, meaning that the only essential input variables are the number of particles and the matrix elements of the Hamiltonian in some single-particle basis set.

Our initial coupled-cluster calculations [35, 36, 37, 38, 39, 40] have focused on closed-shell nuclei. However, the long-term objective of our research program is to study open-shell nuclei with one or more valence nucleons. We would like, for example, to examine how the binding and excitation energies vary with the number of nucleons in valence systems around closed-shell nuclei. This is particularly interesting, when we examine the  $A = 15$  and  $A = 17$  nuclei around  $^{16}\text{O}$ . For example, the splittings between the  $(3/2)_1^-$  and  $(1/2)_1^-$  states in  $^{15}\text{O}$  and  $^{15}\text{N}$  and the splittings between the  $(3/2)_1^+$  and  $(5/2)_1^+$  states in  $^{17}\text{O}$  and  $^{17}\text{F}$  should arise from the nuclear spin-orbit force, which may or may not be affected by three-nucleon interactions. One would like to examine such issues by comparing the results of converged *ab initio* calculations employing two-body interactions with the experimental energy spacings. This requires, however, an appropriate extension of the usual single-reference ground-state

coupled-cluster theory [9, 10, 11, 12] to ground and excited states of valence systems around closed-shell nuclei.

In this paper, we examine, for the first time, the applicability of two quantum-chemistry-inspired coupled-cluster approaches, referred to as the particle-attached (PA) (in chemistry, electron-attached or EA [45, 46, 47, 48, 49]) and particle-removed (PR) (in chemistry, ionized or IP [15, 45, 49, 50, 51, 52, 53, 54, 55]) equation-of-motion coupled-cluster (EOMCC) methods [45, 56, 57], in the converged calculations of the binding and excitation energies of the  $A = 15$  ( $^{15}\text{O}$ ,  $^{15}\text{N}$ ) and  $A = 17$  ( $^{17}\text{O}$ ,  $^{17}\text{F}$ ) nuclei. For these calculations, we use modern nucleon-nucleon interactions derived from the effective-field theory [58, 59], such as  $\text{N}^3\text{LO}$  [30], and their slightly older phenomenological counterparts, including the charge-dependent Bonn interaction model (CD-Bonn) [28] and the  $V_{18}$  model of the Argonne group [27]. In the PA- and PR-EOMCC methods, one calculates ground and excited states of the  $(A + 1)$ - and  $(A - 1)$ -particle systems by diagonalizing the similarity-transformed Hamiltonian of the coupled-cluster theory, resulting from the ground-state calculations for the  $A$ -particle closed-shell nucleus in the relevant  $(A + 1)$ - and  $(A - 1)$ -particle subspaces of the Fock space. As shown in this paper, the PA- and PR-EOMCC approaches provide us with practical computational techniques for potentially accurate *ab initio* studies of valence systems around the closed-shell nuclei that may provide several important insights into the effects of the underlying nucleon-nucleon interactions on the calculated properties of such systems. In addition to the converged PA- and PR-EOMCC results for the  $A = 15$  and  $A = 17$  nuclei obtained with three different types of nucleon-nucleon interactions ( $\text{N}^3\text{LO}$ , CD-Bonn, and  $V_{18}$ ), we provide several details of the PA-EOMCC, PR-EOMCC, and underlying ground-state coupled-cluster calculations, including the factorized forms of the relevant amplitude equations that lead to highly efficient, fully vectorized computer codes applicable to large single-particle basis sets and masses in the  $A \sim 20 - 40$  region.

This paper is divided into four sections. In Sec. II, we present our formalism for deriving an effective two-body Hamiltonian for coupled-cluster calculations, which takes into account short-range nucleon-nucleon correlations, and present the details of the PA-EOMCC and PR-EOMCC theories that enable us to deal with valence systems around closed-shell nuclei within the framework of the single-reference coupled-cluster formalism. The results of PA-EOMCC and PR-EOMCC calculations for the  $^{15}\text{O}$ ,  $^{17}\text{O}$ ,  $^{15}\text{N}$ , and  $^{17}\text{F}$  nuclei are discussed in Sec. III and the conclusions and perspectives are outlined in Sec. IV. The factorized forms of the PA-EOMCC and PR-EOMCC equations for the  $(A \pm 1)$ -particle systems and the corresponding ground-state coupled-cluster equations, exploited in this work, are given in the Appendix.

## II. COUPLED-CLUSTER EQUATIONS FOR VALENCE SYSTEMS

This section serves the aim of presenting the coupled-cluster theories for open-shell nuclei used in this work, with an emphasis on the PA-EOMCC and PR-EOMCC methods mentioned in the Introduction. These methods are designed to handle systems with one valence particle or one valence hole. Since our effective model spaces for the coupled-cluster calculations, which enable us to obtain converged PA-EOMCC and PR-EOMCC results, involve up to eight major harmonic oscillator shells (480 uncoupled single-particle basis states) and 15 to 17 explicitly correlated nucleons, we focus on the computationally efficient formulation of the PA-EOMCC and PR-EOMCC methods that makes such large-scale nuclear structure calculations manageable.

Our theoretical considerations start with the introduction of an appropriate two-body effective interaction for the large-scale coupled-cluster calculations. This is because the majority of modern nucleon-nucleon interactions, including the  $\text{N}^3\text{LO}$ , CD-Bonn, and  $V_{18}$  potentials examined in this study, include repulsive cores that would require calculations in extremely large model spaces to reach converged results [31, 32, 33, 34]. In order to remove the hard-core part of the interaction from the problem and allow for realistic calculations in manageable model spaces with seven or eight major oscillator shells, one has to renormalize the bare interactions. The relevant information about the method used by us to renormalize the  $\text{N}^3\text{LO}$ , CD-Bonn, and  $V_{18}$  Hamiltonians and to generate the final effective Hamiltonians corrected for the center-of-mass contaminations, which can be used in the PA-EOMCC, PR-EOMCC, and other coupled-cluster calculations, are discussed in Sec. II A.

As mentioned in the Introduction, the PA- and PR-EOMCC methods for valence systems are based on an idea of diagonalizing the similarity-transformed Hamiltonian of the coupled-cluster theory, resulting from the ground-state calculations for the  $A$ -particle closed-shell nucleus, in the relevant  $(A + 1)$ - and  $(A - 1)$ -particle subspaces of the Fock space. Thus, before introducing the details of the PA- and PR-EOMCC calculations for the  $(A + 1)$ - and  $(A - 1)$ -particle systems, we provide the most essential information about the underlying closed-shell coupled-cluster calculations that precede the PA- and PR-EOMCC steps. This is done in Sec. II B.

Finally, in Sec. II C, we discuss the most essential details of the PA- and PR-EOMCC calculations for the ground- and excited states of the  $(A + 1)$ - and  $(A - 1)$ -particle valence systems around the closed-shell  $A$ -particle nucleus. The final working equations for the cluster and excitation amplitudes, which define the coupled-cluster, PA-EOMCC, and PR-EOMCC approximations implemented in this work and which lead to highly efficient computer codes, are shown in the Appendix.

### A. Effective Two-Body Interaction for Coupled-Cluster Calculations

In the PR-EOMCC calculations for  $^{15}\text{O}$  and  $^{15}\text{N}$ , the PA-EOMCC calculations for  $^{17}\text{O}$  and  $^{17}\text{F}$ , and the underlying closed-shell coupled-cluster calculations for the ground-state of  $^{16}\text{O}$  which precede the PR-EOMCC and PA-EOMCC calculations, we used the following three nucleon-nucleon interactions:  $\text{N}^3\text{LO}$  [30], CD-Bonn [28], and  $V_{18}$  [27]. The Coulomb interaction was included in all of our calculations (to distinguish between  $^{15}\text{O}/^{17}\text{O}$  and  $^{15}\text{N}/^{17}\text{F}$ ). In order to remove the hard-core part of the interaction, which would require calculations in extremely large model spaces consisting of dozens of major oscillator shells to reach reasonably converged results [31, 32, 33, 34], and enable realistic calculations in manageable model spaces, we follow the procedure exploited in our earlier work [35, 36, 37, 38, 39, 40]. Thus, we renormalize the Hamiltonian through a no-core  $G$ -matrix procedure, described in considerable detail in Refs. [5, 35]. The no-core  $G$ -matrix approach introduces a starting-energy ( $\omega$ ) dependence in the effective two-body matrix elements  $G(\omega)$  defining the renormalized two-body interactions (obtained by analyzing the exactly solvable proton-proton, proton-neutron, and neutron-neutron two-body problems), but much of the  $\omega$  dependence can be eliminated through the use of the Bethe-Brandow-Petschek theorem [61] and the appropriate summation of the class of folded diagrams to infinite order at a given starting energy (see Refs. [5, 35] for further information). For nuclei like  $^{16}\text{O}$ , the dependence on the chosen starting energy  $\omega$  is weak (almost none when seven or eight major oscillator shells are employed [35]). It introduces an uncertainty of 0.1–0.2 MeV per particle for the binding energies.

After renormalizing bare interactions with the  $G$ -matrix approach, our effective Hamiltonian is given by the formula

$$H_{\text{eff}}(\omega) = H_0 + G(\omega), \quad (1)$$

where  $H_0$  is the total kinetic energy of the nucleons. To complete the process of preparing the Hamiltonian for coupled-cluster calculations, we correct the renormalized Hamiltonian  $H_{\text{eff}}(\omega)$ , Eq. (1), resulting from exploiting the no-core  $G$ -matrix procedure, for center-of-mass contaminations using the expression

$$\begin{aligned} H &\equiv H(\omega, \beta_{\text{CoM}}) = H_{\text{eff}}(\omega) + \beta_{\text{CoM}} H_{\text{CoM}} \\ &= z_{\alpha}^{\beta} a^{\alpha} a_{\beta} + \frac{1}{4} v_{\alpha\beta}^{\gamma\delta} a^{\alpha} a^{\beta} a_{\delta} a_{\gamma}, \end{aligned} \quad (2)$$

where  $z_{\alpha}^{\beta} = \langle \alpha | z | \beta \rangle$  and  $v_{\alpha\beta}^{\gamma\delta} = \langle \alpha\beta | v | \gamma\delta \rangle - \langle \alpha\beta | v | \delta\gamma \rangle$  are the relevant one- and two-body matrix elements in a single-particle basis set  $\{|\alpha\rangle\}$  and  $a^{\alpha}$  ( $a_{\alpha}$ ) are the usual creation (annihilation) operators. Here and elsewhere in the present paper, we use the Einstein summation convention over repeated upper and lower indices. The parameter  $\beta_{\text{CoM}}$  is chosen such that the expectation value of

the center-of-mass Hamiltonian  $H_{\text{CoM}}$  with the ground-state coupled-cluster wave function,  $\langle H_{\text{CoM}} \rangle$ , obtained for the  $\beta_{\text{CoM}}$ -dependent Hamiltonian  $H$ , Eq. (2), is 0.0 MeV. This can be done by relying, for example, on the Hellmann-Feynman theorem and calculating  $\langle H_{\text{CoM}} \rangle$  as the first derivative of the coupled-cluster energy with respect to  $\beta_{\text{CoM}}$ . Once we know the values of  $\langle H_{\text{CoM}} \rangle$  at various  $\beta_{\text{CoM}}$  values, we can easily identify the optimum  $\beta_{\text{CoM}}$  value at which  $\langle H_{\text{CoM}} \rangle$  becomes 0.0 MeV [60]. As pointed out in our earlier papers [37, 39, 40], one of the advantages of this procedure is the ease of separation of intrinsic and center-of-mass contaminated states by analyzing the dependence of coupled-cluster energies on  $\beta_{\text{CoM}}$ . As shown in Refs. [39, 40], the physical states obtained in coupled-cluster calculations are virtually independent of  $\beta_{\text{CoM}}$ , while the center-of-mass contaminated states show a strong, nearly linear dependence of excitation energies on  $\beta_{\text{CoM}}$ .

We are currently working on alternative approaches to the effective interaction. In one of these alternatives, instead of relying on the  $G$ -matrix method, we will construct the renormalized Hamiltonian for coupled-cluster calculations with the help of the Lee-Suzuki procedure [62, 63, 64], exploited in the no-core shell-model approach [4]. This procedure will eliminate the starting-energy dependence from our calculations. In particular, we will investigate the differences between our  $G$ -matrix approach and the no-core approach based on the Lee-Suzuki transformation in the forthcoming work. Both methods have the appealing feature that the effective interaction is properly renormalized as the size of the harmonic oscillator basis is increased, approaching the bare Hamiltonian in the limit of an infinite single-particle basis set. We will also study coupled-cluster applications using the  $V_{\text{lowk}}$  effective interaction approach [65]. In this method, one uses the cutoff in momentum space to soften the nucleon-nucleon interaction. The Lee-Suzuki-based and  $G$ -matrix-based no-core procedures rely on the harmonic oscillator basis cutoff only, while the  $V_{\text{lowk}}$  procedure uses the momentum-space cutoff in addition to the basis set cutoff. The three methods will produce identical results in the limit of an infinite basis set and infinite momenta.

Once the one- and two-body matrix elements of the center-of-mass-corrected renormalized Hamiltonian  $H$ , Eq. (2), are determined, we solve the nuclear many-body problem using coupled-cluster theory. In order to construct the coupled-cluster equations for the closed-shell  $A$ -body system and the related PA-EOMCC and PR-EOMCC equations for the  $(A+1)$ - and  $(A-1)$ -body nuclei in the computationally most efficient way, as dictated by the factorized form of these equations discussed in Secs. II B, II C, and the Appendix, we sort the one- and two-body matrix elements of  $H$  according to the particle-hole ( $p$ - $h$ ) character of the single-particle indices that label them prior to the coupled-cluster work. For example, the two-body matrix elements  $v_{\alpha\beta}^{\gamma\delta}$  defining  $H$ , Eq. (2), are sorted out into six groups corresponding to the fol-

lowing  $p$ - $h$  types of single-particle indices  $\alpha, \beta, \gamma, \delta$ :  $hhhh$ ,  $hhhp$ ,  $hhpp$ ,  $hphp$ ,  $hppp$ ,  $pppp$ . The same philosophy of sorting matrix elements according to the  $p$ - $h$  character of the relevant single-particle indices is applied to one- and two-body matrix elements of the similarity-transformed Hamiltonian of coupled-cluster theory discussed in the next subsection. This is a common practice in the most efficient implementations of coupled-cluster methods by quantum chemists and we follow the same recipe here.

### B. Brief Synopsis of the Single-Reference Coupled-Cluster Theory and the Basic CCSD Approximation

As mentioned earlier, the PA-EOMCC and PR-EOMCC calculations for the  $(A+1)$ - and  $(A-1)$ -particle valence systems rely on the diagonalization of the similarity-transformed Hamiltonian, obtained in the single-reference coupled-cluster calculations for the  $A$ -particle closed-shell nucleus, in appropriate subspaces of the Fock space. Thus, before introducing the PA- and PR-EOMCC methods for the  $(A+1)$ - and  $(A-1)$ -particle systems, we provide the most essential information about the underlying closed-shell coupled-cluster calculations that precede the PA- and PR-EOMCC steps.

The single-reference coupled-cluster theory [9, 10, 11, 12] is based on the exponential ansatz for the ground-state wave function of the  $A$ -body system,

$$|\Psi_0^{(A)}\rangle = e^{T^{(A)}}|\Phi\rangle, \quad (3)$$

where  $T^{(A)}$  is the cluster operator (a  $p$ - $h$  excitation operator) and  $|\Phi\rangle$  is the corresponding reference determinant (defining the Fermi vacuum) obtained by performing some mean-field calculation or by simply filling  $A$  lowest-energy single-particle states (this is what we have done in the calculations discussed in this paper). Here and elsewhere in the present paper, we use superscripts, such as  $(A)$ , which indicate the number of particles in a system under consideration, at the relevant operators and energies. Normally, when  $A$  remains fixed throughout the entire calculation, this is not essential, but in this paper we deal with systems with different mass numbers (the  $A$ -body as well as the  $(A+1)$ - and  $(A-1)$ -body systems), so that it is useful to indicate the number of particles in a many-body system of interest at the most essential mathematical quantities to avoid confusion.

Formally, Eq. (3) is a direct consequence of the connected-cluster theorem, first clearly stated by Hubbard [66], which is, in turn, related to the linked cluster theorem of many-body perturbation theory [66, 67, 68, 69]. According to the connected-cluster theorem, the cluster operator  $T^{(A)}$  generates connected wave function diagrams summed through infinite order. Operationally,  $T^{(A)}$  is a simple many-body excitation operator, which in all standard coupled-cluster approximations is truncated at a given (usually low)  $p$ - $h$  excitation level  $M < A$ . An example of the standard coupled-cluster

method is the CCSD (coupled-cluster singles and doubles) approach [70, 71, 72], which is used in this work to obtain the ground-state information for the closed-shell  $^{16}\text{O}$  nucleus. We label coupled-cluster methods by the standard acronyms adopted by chemists who have led the development of coupled-cluster approaches for over 30 years now and they are, by far, the most frequent users of coupled-cluster approaches; see, for example, Refs. [14, 25] for the relevant historical remarks. In this case,  $M = 2$  and the cluster operator  $T^{(A)}$  is approximated by

$$T^{(A)}(\text{CCSD}) \equiv T^{(A)}(2) = T_1 + T_2, \quad (4)$$

where

$$T_1 = t_a^i a^a a_i \quad (5)$$

and

$$T_2 = \frac{1}{4} t_{ab}^{ij} a^a a^b a_j a_i \quad (6)$$

are  $1p$ - $1h$  or singly excited and  $2p$ - $2h$  or doubly excited cluster components,  $t_a^i$  and  $t_{ab}^{ij}$  are the corresponding singly and doubly excited cluster amplitudes, and  $i, j, \dots$  ( $a, b, \dots$ ) are the single-particle states occupied (unoccupied) in the reference determinant  $|\Phi\rangle$ . The general form of the truncated cluster operator, defining a standard single-reference coupled-cluster approximation characterized by the excitation level  $M$ , is

$$T^{(A)}(M) = \sum_{n=1}^M T_n, \quad (7)$$

where

$$T_n = \left(\frac{1}{n!}\right)^2 t_{a_1 \dots a_n}^{i_1 \dots i_n} a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1} \quad (8)$$

( $n = 1, \dots, M$ ) are the many-body components of  $T^{(A)}(M)$ , and  $t_{a_1 \dots a_n}^{i_1 \dots i_n}$  are the corresponding cluster amplitudes.

The cluster amplitudes  $t_{a_1 \dots a_n}^{i_1 \dots i_n}$  are determined by solving a coupled system of nonlinear and energy-independent algebraic equations of the form:

$$\langle \Phi_{i_1 \dots i_n}^{a_1 \dots a_n} | \bar{H}_N(M) | \Phi \rangle = 0, \quad i_1 < \dots < i_n, \quad a_1 < \dots < a_n, \quad (9)$$

where  $n = 1, \dots, M$ ,

$$\bar{H}_N(M) = e^{-T^{(A)}(M)} H_N e^{T^{(A)}(M)} = (H_N e^{T^{(A)}(M)})_C \quad (10)$$

is the similarity-transformed Hamiltonian of the coupled-cluster theory truncated at  $Mp$ - $Mh$  excitations, subscript  $C$  designates the connected part of the corresponding operator expression, and  $|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle \equiv a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1} |\Phi\rangle$  are the  $np$ - $nh$  or  $n$ -tuply excited determinants relative to  $|\Phi\rangle$ . The operator  $H_N$  entering Eq. (10) is the Hamiltonian in the normal-ordered form

relative to the  $A$ -particle Fermi vacuum reference state  $|\Phi\rangle$ ,

$$H_N = H - \langle \Phi | H | \Phi \rangle = f_\alpha^\beta N[a^\alpha a_\beta] + \frac{1}{4} v_{\alpha\beta}^{\gamma\delta} N[a^\alpha a^\beta a_\delta a_\gamma], \quad (11)$$

where  $f_\alpha^\beta \equiv \langle \alpha | f | \beta \rangle = z_\alpha^\beta + v_{\alpha i}^{\beta i}$  are matrix elements of the Fock matrix and  $N[\dots]$  designates the normal product. In particular, the standard CCSD equations for the singly and doubly excited cluster amplitudes  $t_a^i$  and  $t_{ab}^{ij}$ , defining  $T_1$  and  $T_2$ , respectively, can be written as

$$\langle \Phi_i^a | \bar{H}_N(\text{CCSD}) | \Phi \rangle = 0, \quad (12)$$

$$\langle \Phi_{ij}^{ab} | \bar{H}_N(\text{CCSD}) | \Phi \rangle = 0, \quad i < j, \quad a < b, \quad (13)$$

where

$$\begin{aligned} \bar{H}_N(\text{CCSD}) &\equiv \bar{H}_N(2) = e^{-T^{(A)}(\text{CCSD})} H_N e^{T^{(A)}(\text{CCSD})} \\ &= (H_N e^{T^{(A)}(\text{CCSD})})_C \end{aligned} \quad (14)$$

is the similarity-transformed Hamiltonian of the CCSD approach. As mentioned in Sec. II A, we do not use the bare Hamiltonian in our nuclear structure calculations. Thus, the Hamiltonian  $H$  used to construct the similarity-transformed Hamiltonian  $\bar{H}_N(\text{CCSD})$  for the nuclear structure calculations discussed in this paper is replaced by the renormalized form of the Hamiltonian, Eq. (2), resulting from the no-core  $G$ -matrix calculations.

The system of coupled-cluster equations, Eq. (9), is obtained in the following way (suggested by Čížek [11]). We first insert the coupled-cluster wave function  $|\Psi_0^{(A)}\rangle$ , Eq. (3), into the  $A$ -body Schrödinger equation,

$$H_N |\Psi_0^{(A)}\rangle = \Delta E_0^{(A)} |\Psi_0^{(A)}\rangle, \quad (15)$$

where

$$\Delta E_0^{(A)} = E_0^{(A)} - \langle \Phi | H | \Phi \rangle \quad (16)$$

is the corresponding energy relative to the reference energy  $\langle \Phi | H | \Phi \rangle$ , and premultiply both sides of Eq. (15) on the left by  $e^{-T^{(A)}}$  to obtain the connected-cluster form of the Schrödinger equation [11, 13, 19, 73],

$$\bar{H}_N |\Phi\rangle = \Delta E_0^{(A)} |\Phi\rangle, \quad (17)$$

where

$$\bar{H}_N = e^{-T^{(A)}} H_N e^{T^{(A)}} = (H_N e^{T^{(A)}})_C \quad (18)$$

is the similarity-transformed Hamiltonian. Next, we project Eq. (17), in which  $T^{(A)}$  is replaced by its approximate form  $T^{(A)}(M)$ , Eq. (7), onto the excited determinants  $|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle$ , with  $n = 1, \dots, M$ , corresponding to the  $p$ - $h$  excitations included in  $T^{(A)}(M)$ . The excited determinants  $|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle$  are orthogonal to the reference determinant  $|\Phi\rangle$ , so that we end up with the nonlinear

and energy-independent algebraic equations of the form of Eq. (9). Once the system of equations, Eq. (9), is solved for  $T^{(A)}(M)$  or  $t_{a_1 \dots a_n}^{i_1 \dots i_n}$  (or Eqs. (12) and (13) are solved for  $T_1$  and  $T_2$  or  $t_a^i$  and  $t_{ab}^{ij}$ ), the ground-state coupled-cluster energy is calculated using the equation

$$\begin{aligned} E_0^{(A)}(M) &= \langle \Phi | H | \Phi \rangle + \Delta E_0^{(A)}(M) \\ &= \langle \Phi | H | \Phi \rangle + \langle \Phi | \bar{H}_N(M) | \Phi \rangle \\ &= \langle \Phi | H | \Phi \rangle + \langle \Phi | \bar{H}_{N,\text{close}}(M) | \Phi \rangle, \end{aligned} \quad (19)$$

where  $\bar{H}_{N,\text{close}}(M)$  is the closed part of  $\bar{H}_N(M)$  which is represented by those diagrams contributing to  $\bar{H}_N^{(M)}$  that have no external (uncontracted) Fermion lines (as opposed to the open part of  $\bar{H}_N(M)$  which is represented by the diagrams having external or uncontracted Fermion lines; cf. Sec. II C). It can easily be shown that if  $H$  (in our case, the renormalized Hamiltonian defined by Eq. (2)) does not contain higher-than-two-body interactions and  $2 \leq M \leq A$ , we can write

$$E_0^{(A)}(M) = \langle \Phi | H | \Phi \rangle + \langle \Phi | [H_N(T_1 + T_2 + \frac{1}{2}T_1^2)]_C | \Phi \rangle. \quad (20)$$

In other words, we only need  $T_1$  and  $T_2$  clusters to calculate the ground-state energy  $E_0^{(A)}(M)$  of the  $A$ -body ( $A \geq 2$ ) system even if we solve for other cluster components  $T_n$  with  $n > 2$ . Equation (19) can be obtained by projecting the connected-cluster form of the Schrödinger equation, Eq. (17), on the reference configuration  $|\Phi\rangle$  and replacing  $T^{(A)}$  by  $T^{(A)}(M)$ . In fact, the nonlinear character of the system of coupled-cluster equations of the form of Eq. (9) does not mean that the resulting equations contain very high powers of  $T^{(A)}(M)$ . For example, if the Hamiltonian  $H$  (in our case, the renormalized Hamiltonian obtained using the  $G$ -matrix technique) does not contain higher-than-pairwise interactions, the CCSD equations for the  $T_1$  and  $T_2$  clusters, or for the amplitudes  $t_a^i$  and  $t_{ab}^{ij}$  that represent these clusters, become

$$\langle \Phi_i^a | [H_N(1 + T_1 + T_2 + \frac{1}{2}T_1^2 + T_1 T_2 + \frac{1}{6}T_1^3)]_C | \Phi \rangle = 0, \quad (21)$$

$$\begin{aligned} \langle \Phi_{ij}^{ab} | [H_N(1 + T_1 + T_2 + \frac{1}{2}T_1^2 + T_1 T_2 + \frac{1}{6}T_1^3 \\ + \frac{1}{2}T_2^2 + \frac{1}{2}T_1^2 T_2 + \frac{1}{24}T_1^4)]_C | \Phi \rangle = 0. \end{aligned} \quad (22)$$

In general, if the Hamiltonian  $H$  contains two-body interactions only, there are no terms in cluster components  $T_n$  that are higher than quartic terms in the coupled-cluster system, Eq. (9), independent of the truncation scheme  $M$  used to define  $T^{(A)}(M)$ . This is a purely mathematical statement, resulting from the fact that we must connect external lines of  $H_N$  with the vertices representing the many-body components of the cluster operator  $T^{(A)}$  to determine the connected operator product represented by  $\bar{H}_N$ , Eq. (18), and not the result of some arbitrary truncation of the exponential coupled-cluster wave function.

In this work, we apply the CCSD approach to the closed-shell  $^{16}\text{O}$  nucleus and, what is even more important in this particular study, to obtain the corresponding similarity-transformed Hamiltonian  $\bar{H}_N(\text{CCSD})$ , Eq. (14), which is used in the subsequent PR-EOMCC and PA-EOMCC calculations for the ground and excited states of the 15- and 17-particle nuclei. As shown in our earlier papers [35, 36, 37, 38, 39, 40], the CCSD method is perfectly adequate for a highly accurate description of the ground state of  $^{16}\text{O}$ , providing the converged description of the ground state of  $^{16}\text{O}$  for the Hamiltonians containing two-body interactions (the three-body clusters  $T_3$  are negligible [36, 37, 39, 40]). The highly accurate description of the ground state of  $^{16}\text{O}$  is essential for obtaining a well-balanced description of the 15- and 17-particle valence systems around  $^{16}\text{O}$ . The ability of the CCSD approach to provide a highly accurate description of  $^{16}\text{O}$  is also useful from the practical point of view. When properly implemented, the CCSD approach is characterized by the relatively inexpensive  $n_o^2 n_u^4$  steps, where  $n_o$  and  $n_u$  are the numbers of occupied and unoccupied orbitals, respectively, in the single-particle basis set, making it applicable to systems with the larger values of  $A$ . Our codes are already efficient enough to perform the CCSD calculations with  $A \sim 20 - 40$  and up to eight major oscillator shells, which at least for  $A = 16$  is sufficient to obtain the converged description [37].

The explicit and computationally efficient form of the CCSD and other coupled-cluster equations that can be used in routine calculations for many-body systems with larger  $A$  values and larger basis sets, in terms of one- and two-body matrix elements of the (renormalized form of the) Hamiltonian and cluster amplitudes  $t_{a_1 \dots a_n}^{i_1 \dots i_n}$  (in the CCSD case,  $t_a^i$  and  $t_{ab}^{ij}$ ) can be most conveniently derived by applying diagrammatic techniques of many-body theory combined with diagram factorization methods which yield highly vectorized computer codes [23, 35, 42, 43, 44]. Once these equations are properly coded, we solve them using iterative procedures, such as DIIS [74] (see Refs. [43, 75]). The explicitly connected form of the coupled-cluster equations, such as Eqs. (9) or (21) and (22), guarantees that the process of solving these equations leads to connected terms in cluster components  $T_n$  and connected terms in the energy  $E_0^{(A)}(M)$ , independent of the truncation scheme  $M$  used to define  $T^{(A)}(M)$ . The absence of disconnected terms in  $T^{(A)}(M)$  and  $E_0^{(A)}(M)$  is essential to obtain the rigorously size-extensive results. The computationally efficient form of the CCSD equations for the case of pairwise interactions, which can be applied in large-scale nuclear structure calculations such as those discussed in this work, in terms of one- and two-body matrix elements of the similarity-transformed Hamiltonian  $\bar{H}_N(\text{CCSD})$  that serve as the most natural intermediates for setting up these equations and other recursively generated intermediate quantities that are used to obtain a perfectly vectorized computer code, is given in the Appendix.

### C. Equation-of-Motion Coupled-Cluster Methods for Valence Systems: The PA-EOMCCSD and PR-EOMCCSD Approximations and their Implementation for Nuclear Structure Calculations

In addition to providing natural intermediates for setting up coupled-cluster equations, the use of the similarity-transformed Hamiltonians,  $\bar{H}_N(M)$  or  $\bar{H}_N(\text{CCSD})$ , Eqs. (10) or (14), respectively, in coupled-cluster calculations provides a natural mechanism for extending the ground-state coupled-cluster theory to excited states of a given  $A$ -body system or to ground and excited states of the  $(A + k)$ - or  $(A - k)$ -particle systems obtained by attaching  $k$  particles to or removing  $k$  particles from the  $A$ -particle closed-shell core. This can be most efficiently done by exploiting the EOMCC formalism [45, 56, 57] and its PA-EOMCC (in chemistry, EA-EOMCC [45, 46, 47, 48, 49]) and PR-EOMCC (in chemistry, IP-EOMCC [15, 45, 49, 50, 51, 52, 53, 54, 55]) variants, and their various multiply attached and multiply removed or ionized (cf., e.g., Refs. [49, 76, 77, 78]) extensions (see, also, Refs. [79, 80, 81, 82, 83] and [84, 85, 86, 87, 88, 89] for the related linear response and symmetry-adapted cluster configuration interaction formalisms, respectively). In all of these methods, we obtain excited states  $|\Psi_\mu^{(A)}\rangle$  ( $\mu > 0$ ) of the  $A$ -particle system or ground and excited states  $|\Psi_\mu^{(A \pm k)}\rangle$  ( $\mu \geq 0$ ) of the  $A \pm k$ -particle ( $k > 0$ ) systems by applying the suitably defined excitation ( $R_\mu^{(A)}$ ) or particle-attaching/particle-removing ( $R_\mu^{(A \pm k)}$ ) operator to the ground state obtained in the single-reference coupled-cluster calculations for the closed-shell  $A$ -body system. Operators  $R_\mu^{(A)}$  and  $R_\mu^{(A \pm k)}$  are obtained by diagonalizing the similarity-transformed Hamiltonians, such as  $\bar{H}_N(M)$ , Eq. (10), in the case coupled-cluster theory truncated at  $M$ -tuple excitations, or  $\bar{H}_N(\text{CCSD})$ , Eq. (14), in the CCSD case, in the relevant  $A$ -particle and  $(A \pm k)$ -particle subspaces of the Fock space. For example, in the EOMCCSD approximation [56, 57], which is a basic EOMCC approximation for the calculations of excited states of the  $A$ -particle system, we represent excited states  $|\Psi_\mu^{(A)}\rangle$  as

$$|\Psi_\mu^{(A)}\rangle = R_\mu^{(A)} |\Psi_0^{(A)}\rangle = R_\mu^{(A)} e^{T^{(A)}} |\Phi\rangle \quad (23)$$

and replace  $T^{(A)}$  by the cluster operator  $T^{(A)}(\text{CCSD})$ , Eq. (4), obtained in the CCSD calculations, and  $R_\mu^{(A)}$  by

$$R_\mu^{(A)}(\text{CCSD}) \equiv R_\mu^{(A)}(2) = R_{\mu,0} + R_{\mu,1} + R_{\mu,2}, \quad (24)$$

where

$$R_{\mu,0} = r_0 \mathbf{1}, \quad (25)$$

$$R_{\mu,1} = r_a^i a^a a_i, \quad (26)$$

and

$$R_{\mu,2} = \frac{1}{4} r_{ab}^{ij} a^a a^b a_j a_i \quad (27)$$

are the reference,  $1p\text{-}1h$ , and  $2p\text{-}2h$  components of  $R_\mu^{(A)}$  (CCSD), and  $r_0$ ,  $r_a^i$ , and  $r_{ab}^{ij}$  are the corresponding excitation amplitudes ( $\mathbf{1}$  in Eq. (25) is a unit operator). In a more general case of coupled-cluster theory truncated at  $M$ -tuple excitations, where  $T^{(A)}$  is approximated by  $T^{(A)}(M)$ , Eq. (7), the corresponding  $p\text{-}h$  excitation operator  $R_\mu^{(A)}$  in Eq. (23) is approximated by [45]

$$R_\mu^{(A)}(M) = \sum_{n=0}^M R_{\mu,n}, \quad (28)$$

where, in analogy to  $T_n$ ,

$$R_{\mu,n} = \left(\frac{1}{n!}\right)^2 r_{a_1 \dots a_n}^{i_1 \dots i_n} a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1}, \quad (29)$$

for  $n \geq 1$ , and  $R_{\mu,0}$  is defined by Eq. (25). In the EOMCC methods for excited states, sometimes referred to as the EE-EOMCC (excitation energy EOMCC) approaches [45], the  $p\text{-}h$  excitation amplitudes  $r_{a_1 \dots a_n}^{i_1 \dots i_n}$  defining  $R_\mu^{(A)}(M)$  and the corresponding excitation energies  $\omega_\mu^{(A)}(M) = E_\mu^{(A)}(M) - E_0^{(A)}(M)$  of the  $A$ -body system of interest are obtained by diagonalizing the similarity-transformed Hamiltonian  $\bar{H}_N(M)$  or, more precisely, its open part

$$\begin{aligned} \bar{H}_{N,\text{open}}(M) &= (H_N e^{T^{(A)}(M)})_{C,\text{open}} \\ &= e^{-T^{(A)}(M)} H_N e^{T^{(A)}(M)} - \bar{H}_{N,\text{close}}(M) \\ &= e^{-T^{(A)}(M)} H_N e^{T^{(A)}(M)} - \Delta E_0^{(A)}(M), \end{aligned} \quad (30)$$

which has at least two external Fermion lines, in the subspace of the  $A$ -particle Hilbert space spanned by the same excited determinants  $|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle$  with  $n = 1, \dots, M$  that are used to solve the underlying ground-state coupled-cluster calculations ( $\Delta E_0^{(A)}(M)$  in Eq. (30) is the ground-state coupled-cluster energy relative to the reference energy  $\langle \Phi | H | \Phi \rangle$ ; cf. Eq. (16)). In particular, the  $r_a^i$  and  $r_{ab}^{ij}$  amplitudes of the standard EOMCCSD (or EE-EOMCCSD) theory and the corresponding excitation energies  $\omega_\mu^{(A)}$  (CCSD) of the  $A$ -body system are obtained by diagonalizing the open part of the similarity-transformed Hamiltonian of the CCSD approach,

$$\bar{H}_{N,\text{open}}(\text{CCSD}) = (H_N e^{T^{(A)}(\text{CCSD})})_{C,\text{open}}, \quad (31)$$

in the subspace spanned by the singly and doubly excited determinants  $|\Phi_i^a\rangle$  and  $|\Phi_{ij}^{ab}\rangle$  used to set up and solve the ground-state CCSD equations. We used the EOMCCSD approach to calculate the selected excited states of the  $^4\text{He}$  and  $^{16}\text{O}$  nuclei in Refs. [36, 37, 38, 39, 40].

The idea of diagonalizing the similarity-transformed Hamiltonians  $\bar{H}_{N,\text{open}}(M)$ , Eq. (30), or  $\bar{H}_{N,\text{open}}(\text{CCSD})$ , Eq. (31), can be extended to ground and excited states of open-shell nuclei with  $(A \pm k)$  particles by replacing the

particle-conserving  $p\text{-}h$  excitation operator  $R_\mu^{(A)}$  in Eq. (23) by the suitably defined particle-attaching or particle-removing operator  $R_\mu^{(A \pm k)}$ . For example, in the basic PA-EOMCCSD (in chemistry, EA-EOMCCSD) [46, 47] and PR-EOMCCSD (in chemistry, IP-EOMCCSD) [15, 50, 51, 52] approaches (cf., also, Ref. 45, 49) exploited in this work, we define the wave functions of the  $(A+1)$ - and  $(A-1)$ -particle systems, respectively, as

$$|\Psi_\mu^{(A \pm 1)}\rangle = R_\mu^{(A \pm 1)} e^{T^{(A)}} |\Phi\rangle, \quad (32)$$

where  $T^{(A)}$  is approximated by  $T^{(A)}(\text{CCSD})$ , Eq. (4), obtained in the CCSD calculations for the  $A$ -particle closed-shell system, and  $R_\mu^{(A+1)}$  and  $R_\mu^{(A-1)}$  are replaced by the appropriately truncated operators,

$$R_\mu^{(A+1)}(2p\text{-}1h) = R_{\mu,1p} + R_{\mu,2p\text{-}1h} = r_a^i a^a + \frac{1}{2} r_{ab}^{ij} a^a a^b a_j \quad (33)$$

and

$$R_\mu^{(A-1)}(2h\text{-}1p) = R_{\mu,1h} + R_{\mu,2h\text{-}1p} = r^i a_i + \frac{1}{2} r_b^{ij} a^b a_j a_i, \quad (34)$$

respectively, which generate the  $(A+1)$ - and  $(A-1)$ -particle states from the  $A$ -particle CCSD wave function  $e^{T_1+T_2} |\Phi\rangle$ . The  $1p$  and  $2p\text{-}1h$  amplitudes  $r_a^i$  and  $r_{ab}^{ij}$ , respectively, entering Eq. (33) and defining the PA-EOMCCSD model, and the  $1h$  and  $2h\text{-}1p$  amplitudes  $r^i$  and  $r_b^{ij}$ , respectively, entering Eq. (34) and defining the PR-EOMCCSD model, are determined by solving the eigenvalue problem

$$(\bar{H}_{N,\text{open}} R_\mu^{(A \pm 1)})_C |\Phi\rangle = \omega_\mu^{(A \pm 1)} R_\mu^{(A \pm 1)} |\Phi\rangle, \quad (35)$$

where  $\bar{H}_{N,\text{open}}$  is replaced by the similarity-transformed Hamiltonian of the CCSD theory,  $\bar{H}_{N,\text{open}}(\text{CCSD})$ , Eq. (31), in the relevant subspaces of the  $(A+1)$ - and  $(A-1)$ -particle subspaces,  $\mathcal{H}^{(A+1)}$  and  $\mathcal{H}^{(A-1)}$ , respectively, of the Fock space. The subspace of  $\mathcal{H}^{(A+1)}$  used to solve the PA-EOMCCSD eigenvalue problem is spanned by the  $|\Phi^a\rangle = a^a |\Phi\rangle$  and  $|\Phi_{ij}^{ab}\rangle = a^a a^b a_j |\Phi\rangle$  determinants. The subspace of  $\mathcal{H}^{(A-1)}$  used to solve the PR-EOMCCSD problem is spanned by the  $|\Phi_i\rangle = a_i |\Phi\rangle$  and  $|\Phi_{ij}^b\rangle = a^b a_j a_i |\Phi\rangle$  determinants. By solving Eq. (35), we directly obtain the energy differences,  $\omega_\mu^{(A+1)} = E_\mu^{(A+1)} - E_0^{(A)}$  in the PA-EOMCCSD case, and  $\omega_\mu^{(A-1)} = E_\mu^{(A-1)} - E_0^{(A)}$  in the PR-EOMCCSD case, where  $E_\mu^{(A+1)}$  and  $E_\mu^{(A-1)}$  are the energies of ground ( $\mu = 0$ ) and excited ( $\mu > 0$ ) states of the  $(A+1)$ - and  $(A-1)$ -particle systems, respectively, and  $E_0^{(A)}$  is the ground-state coupled-cluster (in this case, CCSD) energy of the  $A$ -particle reference system.

In analogy to the ground-state coupled-cluster theory, one can extend the PA-EOMCCSD and PR-EOMCCSD schemes to higher excitations. For example, in the nuclear analogs of the quantum-chemical EA-EOMCCSDT [48, 49] and IP-EOMCCSDT [49, 53, 54] methods, which we would call here the PA-EOMCCSDT (PA-EOMCC singles, doubles, and triples) and PR-EOMCCSDT (PR-EOMCC singles, doubles, and triples) approaches, one



truncates the ground-state cluster operator  $T^{(A)}$  at the  $3p$ - $3h$  clusters  $T_3$  (the  $M = 3$  or CCSDT case) and augments the  $R_\mu^{(A+1)}(2p$ - $1h)$  and  $R_\mu^{(A-1)}(2h$ - $1p)$  operators, Eqs. (33) and (34), respectively, by the  $3p$ - $2h$  component

$$R_{\mu,3p-2h} = \frac{1}{12} r_{abc}^{jk} a^a a^b a^c a_k a_j, \quad (36)$$

in the  $R_\mu^{(A+1)}$  case, and the  $3h$ - $2p$  component

$$R_{\mu,3h-2p} = \frac{1}{12} r_{bc}^{ijk} a^b a^c a_k a_j a_i \quad (37)$$

in the  $R_\mu^{(A-1)}$  case. The resulting PA-EOMCCSDT and PR-EOMCCSDT operators  $R_\mu^{(A+1)}$  and  $R_\mu^{(A-1)}$  are

$$R_\mu^{(A+1)}(3p-2h) = R_{\mu,1p} + R_{\mu,2p-1h} + R_{\mu,3p-2h} \quad (38)$$

and

$$R_\mu^{(A-1)}(3h-2p) = R_{\mu,1h} + R_{\mu,2h-1p} + R_{\mu,3h-2p}, \quad (39)$$

respectively. In general, if the cluster operator  $T^{(A)}$  defining the ground-state of the  $A$ -body system is truncated at the  $Mp$ - $Mh$  component, as shown in Eq. (7), one typically truncates the corresponding PA-EOMCC operator  $R_\mu^{(A+1)}$  and the corresponding PR-EOMCC operator  $R_\mu^{(A-1)}$  as follows:

$$R_\mu^{(A+1)} = \sum_{n=0}^{M-1} R_{\mu,(n+1)p-nh}, \quad (40)$$

where

$$R_{\mu,(n+1)p-nh} = \frac{1}{n!(n+1)!} r_{aa_1 \dots a_n}^{i_1 \dots i_n} \times a^a a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1} \quad (41)$$

and

$$R_\mu^{(A-1)} = \sum_{n=0}^{M-1} R_{\mu,(n+1)h-np}, \quad (42)$$

where

$$R_{\mu,(n+1)h-np} = \frac{1}{n!(n+1)!} r_{a_1 \dots a_n}^{ii_1 \dots i_n} \times a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1} a_i, \quad (43)$$

although, at least in principle, one could extend the summations over  $n$  in Eqs. (40) and (42) to  $\sum_{n=0}^M$  without affecting the explicit connectedness of the left-hand side of the corresponding PA-EOMCC and PR-EOMCC eigenvalue problems, Eq. (35). The detailed discussion of the relationships between truncation schemes in the  $R_\mu^{(A\pm 1)}$  and  $T^{(A)}$  operators in the PA-EOMCC or EA-EOMCC and PR-EOMCC or IP-EOMCC calculations can be found in Ref. [45] (cf.,

also, Refs. [49, 90] for additional comments and numerical tests). The  $(n+1)p$ - $nh$  and  $(n+1)h$ - $np$  amplitudes  $r_{aa_1 \dots a_n}^{i_1 \dots i_n}$  and  $r_{a_1 \dots a_n}^{ii_1 \dots i_n}$ , entering the  $R_\mu^{(A+1)}$  and  $R_\mu^{(A-1)}$  operators of Eqs. (40) and (42), respectively, are obtained by solving the eigenvalue problem defined by Eq. (35), in which  $\bar{H}_{N,\text{open}}$  is replaced by  $\bar{H}_N(M)$ , Eq. (10). The subspace of  $\mathcal{H}^{(A+1)}$  relevant to the corresponding truncated PA-EOMCC problem is spanned by the  $|\Phi^a\rangle$  and  $|\Phi_{i_1 \dots i_n}^{aa_1 \dots a_n}\rangle = a^a a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1} |\Phi\rangle$  ( $n = 1, \dots, M-1$ ) determinants. Similarly, the subspace of  $\mathcal{H}^{(A-1)}$  relevant to the corresponding truncated PR-EOMCC problem is spanned by the  $|\Phi_i\rangle$  and  $|\Phi_{ii_1 \dots i_n}^{a_1 \dots a_n}\rangle = a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1} a_i |\Phi\rangle$  ( $n = 1, \dots, M-1$ ) determinants.

The PA-EOMCC and PR-EOMCC methods, as described above, and their extensions to two or more valence particle or holes via multiply attached or multiply ionized schemes [49, 76, 77, 78] offer several advantages compared to the equally accurate, but usually a lot more complicated, genuine multi-reference coupled-cluster methods of either the valence-universal [91, 92] or the Hilbert-space or state-universal [93] type that are specifically designed to handle general classes of open-shell problems. Although there has been significant progress in recent years in the development of genuine multi-reference coupled-cluster theories [94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106], multi-reference coupled-cluster calculations are often plagued by intruder states, unphysical, singular, and multiple solutions, and mathematical difficulties with the proper adaptation of the corresponding equations to symmetries of the Hamiltonian if one aims at the general-purpose computer codes (cf., e.g., Refs. [95, 107, 108, 109, 110, 111, 112, 113, 114] for further information). Some of these issues are currently being addressed (cf., e.g., Refs. [97, 98, 99, 100, 101, 102, 103, 104, 106]), but none of these problems are present in the PA-EOMCC and PR-EOMCC calculations, which could be viewed as the physically motivated, intruder-state free, state-selective modifications of the powerful and elegant valence-universal multi-reference coupled-cluster schemes pioneered by Mukherjee and Lindgren [91, 92]. In particular, the use of the similarity-transformed Hamiltonian  $\bar{H}_{N,\text{open}}$  obtained in the coupled-cluster calculations for an  $A$ -particle closed-shell system, which commutes with the symmetry operators of the original Hamiltonian  $H$ , automatically guarantees that the PA-EOMCC and PR-EOMCC wave functions defined by Eq. (32), obtained by diagonalizing  $\bar{H}_{N,\text{open}}$  in the appropriate subspaces of  $\mathcal{H}^{(A+1)}$  and  $\mathcal{H}^{(A-1)}$ , are automatically adapted to the symmetries of the Hamiltonian  $H$  and one does not have to worry about the symmetry-contamination issues facing the implementations of the open-shell coupled-cluster schemes employing the unrestricted reference determinants.

Our calculations for the ground and low-lying excited states of the 15- and 17-particle nuclei around  $^{16}\text{O}$ , reported in this work, have been performed with the basic

PA-EOMCCSD and PR-EOMCCSD methods, in which the ground-state of  $^{16}\text{O}$  is represented by the CCSD wave function  $e^{T_1+T_2}|\Phi\rangle$  and the nucleon-attaching and nucleon-removing operators  $R_\mu^{(A+1)}$  and  $R_\mu^{(A-1)}$  are defined by Eqs. (33) and (34), respectively. We can obtain an accurate description of the  $(A+1)$ -particle nuclei  $^{17}\text{O}$  and  $^{17}\text{F}$  with the PA-EOMCCSD method, in which we include the  $1p$  and  $2p-1h$  excitations from the  $^{16}\text{O}$  core to form the 17-particle systems, since the ground-states and the low-lying excited states of the  $^{17}\text{O}$  and  $^{17}\text{F}$  nuclei that we have singled out in this work are essentially one-quasi-particle states, except, perhaps, for the  $(3/2)_1^+$  states of  $^{17}\text{O}$  and  $^{17}\text{F}$ , which are resonances. Similarly, we can study the  $(A-1)$ -particle nuclei  $^{15}\text{O}$  and  $^{15}\text{N}$  with the basic PR-EOMCCSD approach, in which we include the  $1h$  and  $2h-1p$  excitations from the  $^{16}\text{O}$  closed-shell core, since the low-lying states of these nuclei are expected to be dominated by one-quasi-hole states with respect to the  $A$ -body reference  $^{16}\text{O}$  nucleus. As discussed in Ref. [1], there is, for example, almost no experimental evidence for the fragmentation of the quasi-hole  $p_{1/2}$  and  $p_{3/2}$  states of  $^{16}\text{O}$ . The fact that we use the  $1p$  and  $2p-1h$  excitations in the PA-EOMCCSD calculations to form the  $(A+1)$ -body systems and the fact that we use the  $1h$  and  $2h-1p$  excitations in the PR-EOMCCSD calculations for the  $(A-1)$ -body systems mean that we include many of the same correlations as Fujii *et al.* [115, 116]. Their approach is analogous to a hermitian coupled-cluster approach (see Ref. [116]). There are, however, differences between our PA-EOMCCSD and PR-EOMCCSD calculations and the calculations reported by Fujii *et al.* We use a biorthogonal EOMCC formalism, based on diagonalizing the non-hermitian similarity-transformed Hamiltonian  $\bar{H}_N(\text{CCSD})$ , Eq. (14), obtained in highly accurate CCSD calculations for the  $A$ -body closed-shell nucleus, which has been very successful in quantum chemistry and molecular physics and which brings a lot of correlations within basic truncation schemes, such as EOMCCSD, PA-EOMCCSD, and PR-EOMCCSD, through the presence of high-order correlation terms in  $\bar{H}_N(\text{CCSD})$ . We also differ in the definition of the model space, since Fujii *et al.* use a model space similar to that used in the no-core shell-model calculations [4], in which a “triangular” energy cutoff is applied to Slater determinants included in the diagonalization of the Hamiltonian, in addition to the usual single-particle basis set cutoff. Such a model space cannot be used in coupled-cluster calculations since it violates the Pauli principle in the summations over the intermediate states that emerge through products of many-body components of the cluster operator  $T^{(A)}$  in coupled-cluster equations. As mentioned earlier, the use of a given truncation scheme for the cluster operator  $T^{(A)}$  implies specific truncation schemes for the EOMCC operators, such as  $R_\mu^{(A+1)}$  and  $R_\mu^{(A-1)}$ . Thus, we use all  $1p$  and  $2p-1h$  or  $1h$  and  $2h-1p$  excitations in the PA-EOMCCSD and PR-EOMCCSD calculations and all  $1p-1h$  and  $2p-2h$  cluster amplitudes  $t_a^i$  and  $t_{ab}^{ij}$  that are allowed by a given single-particle basis set, without im-

posing additional energy cutoffs on the determinants that these excitations correspond to, producing many additional and important correlations that are outside model spaces used in the no-core shell-model calculations.

The use of the CCSD method for describing the correlated ground-state of the  $^{16}\text{O}$  reference nucleus in the PR-EOMCCSD and PA-EOMCCSD calculations for the 15- and 17-particle systems around  $^{16}\text{O}$  is justified by the virtually perfect agreement of the CCSD results and the results of the exact shell-model diagonalization of the Hamiltonian in the same model space as used in the CCSD calculations [36, 117]. As shown in Refs. [37, 39, 40] (cf., also, Ref. [117]), the three-body clusters  $T_3$  play a negligible role in the calculations of the binding energy of  $^{16}\text{O}$  when the Hamiltonian includes pairwise interactions. They also have almost no effect on the lowest-energy  $J^\pi = 3^-$  state of  $^{16}\text{O}$ , which is dominated by the  $1p-1h$  excitations, if the Hamiltonian contains the two-body interactions only [37, 39, 40]. In this case, the basic EOMCCSD method, defined by Eq. (23) in which  $T^{(A)}$  is replaced by the CCSD operator  $T^{(A)}(\text{CCSD})$ , Eq. (4), and  $R_\mu^{(A)}$  is defined by Eq. (24), provides the virtually converged description. Interestingly enough, our PA-EOMCCSD and PR-EOMCCSD results for the binding energies of  $^{17}\text{O}/^{17}\text{F}$  and  $^{15}\text{O}/^{15}\text{N}$ , reported in this work, enable us to explain most of the 6 MeV difference between the converged coupled-cluster and experimental results for the lowest  $J^\pi = 3^-$  state of  $^{16}\text{O}$ , reported, for example, in Ref. [37], which, according to our analysis, may largely be caused by the three-body interactions neglected in our calculations that affect the relevant single-particle energy spacings (see Sec. III B for a detailed discussion).

If we were to incorporate  $T_3$  components in the ground-state coupled-cluster calculations for  $^{16}\text{O}$ , we would also have to include the  $3p-2h$  excitations  $R_{\mu,3p-2h}$ , Eq. (36), in the calculations for the 17-particle nuclei and the  $3h-2p$  excitations  $R_{\mu,3h-2p}$ , Eq. (37), in the calculations for the 15-particle nuclei. Although we do not expect the  $R_{\mu,3p-2h}$  and  $R_{\mu,3h-2p}$  terms to be significant for the calculations discussed in this work, we will examine their role in the future work, once the corresponding highly efficient computer codes for large-scale nuclear applications are developed. As explained in Refs. [45, 49], it is formally possible to include the  $R_{\mu,3p-2h}$  and  $R_{\mu,3h-2p}$  components in the PA-EOMCCSD and PR-EOMCCSD approaches, which are then called the PA-EOMCCSD( $3p-2h$ ) and PR-EOMCCSD( $3h-2p$ ) methods, respectively [49], without losing the explicitly connected form of the left-hand side of the corresponding PA-EOMCC and PR-EOMCC eigenvalue problems given by Eq. (35). A promising new development in the area of including the relatively expensive  $R_{\mu,3p-2h}$  and  $R_{\mu,3h-2p}$  terms in the PA-EOMCC and PR-EOMCC methods is that of the so-called active-space PA-EOMCC (EA-EOMCC) and PR-EOMCC (IP-EOMCC) approaches, which enable one to reduce the costs of the corresponding parent PA-EOMCCSDT (or EA-EOMCCSDT), PR-

EOMCCSDT (or IP-EOMCCSDT), and other more expensive higher-order PA-EOMCC and PR-EOMCC calculations through a small subset of active single-particle states, which in the nuclear physics context would correspond to the highest occupied and lowest unoccupied shells of the  $A$ -body reference nucleus (see Ref. [49] for details). We will investigate the effects of the  $3p$ - $2h$  and  $3h$ - $2p$  excitations on the PA-EOMCCSD and PR-EOMCCSD results for  $^{15}\text{O}$ ,  $^{17}\text{O}$ ,  $^{15}\text{N}$ , and  $^{17}\text{F}$  reported in this study using the PA-EOMCCSD( $3p$ - $2h$ ), PR-EOMCCSD( $3h$ - $2p$ ) approaches and the active-space variants of the PA-EOMCCSDT and PR-EOMCCSDT methods of Ref. [49] in our future works.

We end this section by presenting the most essential algorithmic details of the highly efficient PA-EOMCCSD and PR-EOMCCSD computer codes that can be applied to valence systems with one valence particle and one valence hole around the closed shell nucleus, such as  $^{16}\text{O}$ , and other computational details pertinent to the specific calculations for the  $^{15}\text{O}$ ,  $^{17}\text{O}$ ,  $^{15}\text{N}$ , and  $^{17}\text{F}$  nuclei discussed in this paper. First, as discussed in Sec. II A, we compute a  $G$  matrix in a harmonic oscillator basis. In the case of the calculations for the 15–17-particle systems described in this paper, we used model spaces consisting of five to eight major oscillator shells; the  $G$  matrix and its pertinent two-body effective interaction were computed for oscillator energies in the range  $\hbar\Omega \in [10, 20]$  MeV and the optimum  $\hbar\Omega$  value for each single-particle basis set was determined by finding the minimum on the curve representing the dependence of the CCSD ground-state energy of  $^{16}\text{O}$  on  $\hbar\Omega$  (see Ref. [35] for the details). The renormalized Hamiltonian resulting from the  $G$  matrix calculations was corrected for the spurious center-of-mass motion using Eq. (2), in which  $\beta_{\text{CoM}}$  was chosen such that the expectation value of the center-of-mass Hamiltonian  $H_{\text{CoM}}$  with the ground-state CCSD wave function of  $^{16}\text{O}$  is 0.0 MeV. Since the PA-EOMCCSD and PR-EOMCCSD methods are based on the linear-response-like idea of directly calculating the energy differences  $\omega_{\mu}^{(A\pm 1)} = E_{\mu}^{(A\pm 1)} - E_0^{(A)}$  between the  $(A \pm 1)$ - and  $A$ -particle systems rather than the total energies themselves, where the ground-state of the closed-shell  $A$ -particle system serves as a reference for the  $(A \pm 1)$ -body systems and where we diagonalize the similarity-transformed Hamiltonian obtained in the CCSD calculations for the  $A$ -particle reference system, we used the optimum values of  $\hbar\Omega$  and  $\beta_{\text{CoM}}$  determined for  $^{16}\text{O}$  in the final PA-EOMCCSD and PR-EOMCCSD calculations for  $^{15}\text{O}$ ,  $^{17}\text{O}$ ,  $^{15}\text{N}$ , and  $^{17}\text{F}$  reported in this paper. As already mentioned, for larger single-particle basis sets with seven or eight major oscillator shells, the dependence of the results on  $\hbar\Omega$  is virtually none. The dependence of the energies of physical states on  $\beta_{\text{CoM}}$  is virtually none as well (cf. Refs. [35, 37, 38, 39, 40] for the details). Thus, the specific values of  $\hbar\Omega$  and  $\beta_{\text{CoM}}$  become less and less important when the physical states are identified and when larger basis sets are employed (in fact, the optimum  $\beta_{\text{CoM}}$  values approach zero as the basis

set increases; cf. Table I). Most of our calculations for  $^{15}\text{O}$ ,  $^{17}\text{O}$ ,  $^{15}\text{N}$ , and  $^{17}\text{F}$  were based on the  $\text{N}^3\text{LO}$  nucleon-nucleon interaction model of Machleidt and co-workers [30], although we also performed the calculations for the CD-Bonn interaction model [28] and the  $V_{18}$  model of the Argonne group [27]. As pointed out earlier, the Coulomb interaction was included in all of the calculations.

Once the one- and two-body matrix elements of the center-of-mass-corrected effective Hamiltonian, Eq. (2), are determined and properly sorted out, as described in Sec. II A, we set up and solve the CCSD equations for the closed-shell  $A$ -particle system (in our case,  $^{16}\text{O}$ ), the PA-EOMCCSD equations for the  $(A+1)$ -particle systems ( $^{17}\text{O}$  and  $^{17}\text{F}$ ), and the PR-EOMCCSD equations for the  $(A-1)$ -particle systems ( $^{15}\text{O}$  and  $^{15}\text{N}$ ). Our ground-state CCSD computer codes rely on the DIIS solver [74] (see, also, Refs. [43, 75]), whereas the PA-EOMCCSD and PR-EOMCCSD equations for ground and excited states of the  $(A+1)$ - and  $(A-1)$ -particle nuclei are solved with the Hirao-Nakatsuji generalization [118] of the Davidson diagonalization algorithm [119] to nonhermitian eigenvalue problems. The computationally efficient form of the CCSD equations in terms of recursively generated intermediates can be derived diagrammatically using Eqs. (21) and (22). From the point of view of code efficiency, it is important to realize that some of the intermediates entering the CCSD and other CCSD-based equations represent matrix elements of the one- and two-body components of the CCSD similarity-transformed Hamiltonian  $\bar{H}_{N,\text{open}}(\text{CCSD})$ , Eq. (31). If  $\bar{H}_n$  is the  $n$ -body component of  $\bar{H}_{N,\text{open}}^{(\text{CCSD})}$ , for the one- and two-body components  $\bar{H}_1$  and  $\bar{H}_2$ , respectively, we can write

$$\bar{H}_1 = \bar{h}_{\alpha}^{\beta} N[a^{\alpha} a_{\beta}] \quad (44)$$

and

$$\bar{H}_2 = \frac{1}{4} \bar{h}_{\alpha\beta}^{\gamma\delta} N[a^{\alpha} a^{\beta} a_{\delta} a_{\gamma}], \quad (45)$$

where  $\bar{h}_{\alpha}^{\beta}$  and  $\bar{h}_{\alpha\beta}^{\gamma\delta}$  are the one- and two-body matrix elements of  $\bar{H}_{N,\text{open}}^{(\text{CCSD})}$  that enter the CCSD, PA-EOMCCSD, and PR-EOMCCSD equations. As shown in the Appendix, matrix elements  $\bar{h}_{\alpha}^{\beta}$  and  $\bar{h}_{\alpha\beta}^{\gamma\delta}$  are calculated using the one- and two-body matrix elements of the Hamiltonian in the normal-ordered form,  $f_{\alpha}^{\beta}$  and  $v_{\alpha\beta}^{\gamma\delta}$ , respectively (cf. Eq. 11)) and the singly and doubly excited cluster amplitudes  $t_a^i$  and  $t_{ab}^{ij}$ , defining  $T_1$  and  $T_2$ , respectively. The computationally efficient form of the CCSD equations for the case of pairwise interactions in  $H$ , in terms of selected types of  $\bar{h}_{\alpha}^{\beta}$  and  $\bar{h}_{\alpha\beta}^{\gamma\delta}$  and other recursively generated intermediates is given in the Appendix.

We also give in the Appendix the computationally efficient form of the equations defining the PA-EOMCCSD and PR-EOMCCSD eigenvalue problems. These are obtained by applying diagrammatic methods to the PA-EOMCCSD and PR-EOMCCSD equations, which can

be given the following general form:

$$\begin{aligned} \langle \Phi^a | [(\bar{H}_1 R_{\mu,1p})_C + \sum_{n=1}^2 (\bar{H}_n R_{\mu,2p-1h})_C] | \Phi \rangle \\ = \omega_\mu^{(A+1)} r_a, \end{aligned} \quad (46)$$

$$\begin{aligned} \langle \Phi_{ij}^{ab} | [(\bar{H}_2 R_{\mu,1p})_C + \sum_{n=1}^3 (\bar{H}_n R_{\mu,2p-1h})_C] | \Phi \rangle \\ = \omega_\mu^{(A+1)} r_{ab}^j, \end{aligned} \quad (47)$$

in the PA-EOMCCSD case, and

$$\begin{aligned} \langle \Phi_i | [(\bar{H}_1 R_{\mu,1h})_C + \sum_{n=1}^2 (\bar{H}_n R_{\mu,2h-1p})_C] | \Phi \rangle \\ = \omega_\mu^{(A-1)} r^i, \end{aligned} \quad (48)$$

$$\begin{aligned} \langle \Phi_{ij}^b | [(\bar{H}_2 R_{\mu,1h})_C + \sum_{n=1}^3 (\bar{H}_n R_{\mu,2h-1p})_C] | \Phi \rangle \\ = \omega_\mu^{(A-1)} r_{ij}^b, \end{aligned} \quad (49)$$

in the PR-EOMCCSD case. Although formally the PA-EOMCCSD and PR-EOMCCSD equations require the consideration of the three-body components of  $\bar{H}_{N,\text{open}}^{(\text{CCSD})}$  (cf. the  $n = 3$  terms in Eqs. (47) and (49)), we do not have to calculate the corresponding six-index matrix elements  $\bar{h}_{\alpha\beta\gamma}^{\delta\epsilon\eta}$  explicitly. With the help of diagrammatic techniques, the three-body components of  $\bar{H}_{N,\text{open}}^{(\text{CCSD})}$  that enter the PA-EOMCCSD and PR-EOMCCSD equations can be rigorously factorized and rewritten in terms of the one- and two-body components of  $\bar{H}_{N,\text{open}}^{(\text{CCSD})}$ . In consequence, the final working equations of the PA-EOMCCSD and PR-EOMCCSD methods in terms of one- and two-body matrix elements of the Hamiltonian,  $f_\alpha^\beta$  and  $v_{\alpha\beta}^{\gamma\delta}$ , respectively,  $T_1$  and  $T_2$  cluster amplitudes defining the underlying  $A$ -particle ground-state CCSD problem, and the  $R_{\mu,1p}$ ,  $R_{\mu,2p-1h}$ ,  $R_{\mu,1h}$ , and  $R_{\mu,2h-1p}$  excitation amplitudes defining the particle-attaching and particle-removing operators,  $R_\mu^{(A+1)}(2p-1h)$  and  $R_\mu^{(A-1)}(2h-1p)$ , respectively, can be re-expressed in terms of the one- and two-body matrix elements of  $\bar{H}_{N,\text{open}}^{(\text{CCSD})}$ ,  $\bar{h}_\alpha^\beta$  and  $\bar{h}_{\alpha\beta}^{\gamma\delta}$ , respectively, and a few additional recursively generated intermediates, leading to a fully vectorizable algorithm. This computationally efficient form of the PA-EOMCCSD and PR-EOMCCSD equations is given in the Appendix too.

In addition to code vectorization, the main advantage of deriving the CCSD, PA-EOMCCSD, and PR-EOMCCSD equations in the form shown in the Appendix is the possibility of obtaining the relatively low CPU operation count that characterizes these methods. The CCSD equations and the determination of the full set of one- and two-body matrix elements of  $\bar{H}_{N,\text{open}}^{(\text{CCSD})}$  are characterized by the  $n_o^2 n_u^4$  steps, where, as mentioned earlier,  $n_o$  and  $n_u$  are the numbers of occupied and unoccupied orbitals, respectively, in the single-particle basis set.

Once the CCSD equations are solved and all one- and two-body matrix elements of  $\bar{H}_{N,\text{open}}^{(\text{CCSD})}$  are determined, the most expensive steps of the PA-EOMCCSD and PR-EOMCCSD methods employing the factorized equations shown in the Appendix are  $n_o n_u^4$  and  $n_o^2 n_u^3$ , respectively. These relatively low,  $\mathcal{N}^5 - \mathcal{N}^6$  scalings of the costs of the CCSD, PA-EOMCCSD, and PR-EOMCCSD calculations with the system size ( $\mathcal{N}$ ), which are often orders of magnitude smaller than the costs of shell-model calculations aimed at similar accuracies, are among the most important advantages of the coupled-cluster methodology pursued in this work.

### III. RESULTS AND DISCUSSION

#### A. Results of the PR-EOMCCSD and PA-EOMCCSD Calculations with the $N^3\text{LO}$ Interaction and their Convergence with the Basis Set

We focus first on the convergence of our PR-EOMCCSD and PA-EOMCCSD results for the ground and excited states of  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$  and  $^{17}\text{F}$  with the size of the single-particle basis set used in the coupled-cluster calculations (see Tables I and II) and address the issue of the dependence of these results on the choice of the oscillator parameter  $\hbar\Omega$ . For comparison purposes, we also list our previously published ground-state CCSD results for  $^{16}\text{O}$  [37] (cf. Table I), since  $^{16}\text{O}$  serves as a reference nucleus for the PR-EOMCCSD and PA-EOMCCSD calculations. We limit our discussion of the convergence properties of the PR-EOMCCSD and PA-EOMCCSD results for  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$ , and  $^{17}\text{F}$  to the  $N^3\text{LO}$  interaction model [30]. The PR-EOMCCSD and PA-EOMCCSD results for the CD-Bonn [28] and Argonne  $V_{18}$  [27] interactions exhibit almost identical qualitative features in terms of their convergence with the number of major oscillator shells and the way they depend on  $\hbar\Omega$ .

As shown in Table I, the PR-EOMCCSD binding energies of  $^{15}\text{O}$  and  $^{15}\text{N}$ , the results of the CCSD calculations for the binding energy of  $^{16}\text{O}$ , and the PA-EOMCCSD binding energies of  $^{17}\text{O}$  and  $^{17}\text{F}$  are practically converged at the level of eight major oscillator shells. As demonstrated earlier for  $^{16}\text{O}$  [35], the dependence of these results on the oscillator energy  $\hbar\Omega \in [10, 20]$  MeV is almost negligible, particularly for seven or eight major oscillator shells. In the latter case, the dependence of the results on  $\hbar\Omega$  is practically none. This tells us that the renormalization of the short-range part of the nucleon-nucleon interaction with the no-core  $G$ -matrix approach combined with the inclusion of singly and doubly excited clusters and the corresponding  $1p$ ,  $2p-1h$ ,  $1h$ , and  $2h-1p$  excitations in the coupled-cluster and PR-EOMCC/PA-EOMCC calculations for the valence systems around  $^{16}\text{O}$  leads to reasonably well converged ground-state energies of these systems. It is true that the  $N^3\text{LO}$  interaction model has a rather soft core, since it carries a cutoff in

TABLE I: Total binding energies and binding energies per particle (in parentheses) for  $^{15}\text{O}$  and  $^{15}\text{N}$  (the PR-EOMCCSD values),  $^{16}\text{O}$  (the CCSD values), and  $^{17}\text{O}$  and  $^{17}\text{F}$  (the PA-EOMCCSD values), computed with the  $\text{N}^3\text{LO}$  interaction model [30], as functions of the number of major oscillator shells  $N$ . All entries (except for the unitless parameter  $\beta_{\text{CoM}}$ ) are in MeV. The results for  $^{16}\text{O}$  are taken from Ref. [37]. The acronym Expt stands for the experimental values, taken from Ref. [120]. All energies were calculated at the optimum values of  $\hbar\Omega$  (the second last row; determined by identifying the  $\hbar\Omega$  value at which the CCSD energy of  $^{16}\text{O}$  reaches the minimum value) and  $\beta_{\text{CoM}}$  (the last row; determined by the condition that the expectation value of  $H_{\text{CoM}}$  with the CCSD wave function is 0.0 MeV). For eight major oscillator shells, the results are virtually independent of  $\hbar\Omega$  and  $\beta_{\text{CoM}} = 0.0$ .

Nucleus	$N = 5$	$N = 6$	$N = 7$	$N = 8$	Expt
$^{15}\text{O}$	91.047 (6.070)	93.772 (6.251)	93.219 (6.215)	92.376 (6.158)	111.955 (7.464)
$^{15}\text{N}$	94.127 (6.275)	96.432 (6.429)	95.685 (6.379)	95.086 (6.339)	115.492 (7.699)
$^{16}\text{O}$	108.943 (6.810)	113.341 (7.084)	112.446 (7.028)	111.221 (6.951)	127.619 (7.976)
$^{17}\text{O}$	109.218 (6.425)	115.534 (6.796)	115.327 (6.784)	114.277 (6.722)	131.762 (7.751)
$^{17}\text{F}$	106.097 (6.241)	112.869 (6.640)	112.782 (6.634)	111.510 (6.559)	128.220 (7.542)
$\hbar\Omega$	13	11	10	11	
$\beta_{\text{CoM}}$	1.50	0.15	0.05	0.0	

relative momentum of  $\Lambda = 500$  MeV. Thus, in developing the effective two-body interaction based on  $\text{N}^3\text{LO}$  by diagonalizing the deuteron in an oscillator basis, one obtains a converged result to six leading digits with 50 to 60 oscillator shells for  $\hbar\Omega \in [5, 50]$  MeV. For the CD-Bonn and  $V_{18}$  interactions, one needs more than 100 major shells in order to obtain a converged result for the deuteron. However, the advantage of the  $G$ -matrix approach used in this work is that we can renormalize the short-range part of the interaction exactly, since the free part of the  $G$  matrix is computed in a momentum basis first, with the relative momenta  $|\mathbf{p}| \in [0, \infty)$ . Thus, the renormalization problems of the short-range part of the two-body interaction, seen, for example, in the no-core approach [4], with a relatively slow convergence as a function of the harmonic oscillator excitations, are not present here. This means, in turn, that when we use this  $G$  matrix in coupled-cluster calculations, the results for all modern nucleon-nucleon potentials, such as  $\text{N}^3\text{LO}$ , CD-Bonn, and  $V_{18}$  used here, are basically converged within eight major shells. It should also be pointed out that our results for  $\text{N}^3\text{LO}$  agree very well with those of Fujii *et al.* [115].

The fact that our  $G$ -matrix-based coupled-cluster results are essentially converged with the basis set has several important consequences for nuclear many-body the-

ory. We can, for example, claim that any disagreements with experimental data are, most likely, due to the missing degrees of freedom in our Hamiltonians, such as three-nucleon interactions. Indeed, as shown in Table I, our coupled-cluster calculations miss the experimental binding energies (taken from Ref. [120]) by approximately 1.3 – 1.4 MeV per nucleon for the  $A = 15$  nuclei and by approximately 1 MeV per nucleon for the  $A = 16$  and  $A = 17$  systems. At least in principle, several factors can contribute to these differences, but we believe that the three-body interactions are the primary source. It is true, for example, that we are using the solution to a two-body problem (our  $G$  matrix) as the starting point for defining a many-body Hamiltonian with pairwise interactions for the  $A = 15 - 17$  nuclei, and it is known that a two-body interaction derived from the diagonalization of a three-body problem is different from the corresponding two-body interaction derived by diagonalizing the two-body problem (e.g., deuteron) [4, 121, 122]. However, as the size of the model space is increased, both two-body interactions yield very similar results (see the discussion in Ref. [121]). Thus, since we use large model spaces with seven or even eight major oscillator shells, the differences between these two types of effective two-body interactions are minimal and cannot, as such, contribute to the differences between the coupled-cluster and experimental data observed in our calculations. Clearly, we are missing some correlations in our coupled-cluster calculations, which ignore, for example,  $T_3$  clusters in the ground-state calculations for  $^{16}\text{O}$  and  $3p\text{-}2h$  and  $3h\text{-}2p$  components of  $R_\mu^{(A+1)}$  and  $R_\mu^{(A-1)}$  in the PR-EOMCC and PA-EOMCC calculations for the 15- and 17-particle nuclei, but, as mentioned earlier, the ground and excited states of  $^{15}\text{O}/^{15}\text{N}$  and  $^{17}\text{O}/^{17}\text{F}$  are essentially one-quasi-particle and one-quasi-hole states, respectively, in which  $3p\text{-}2h$  and  $3h\text{-}2p$  excitations play a negligible role. As shown in Refs. [37, 39, 40],  $T_3$  clusters bring in at most a total of 1 MeV in the ground-state calculations for  $^{16}\text{O}$  (less than 0.1 MeV per nucleon) and cannot, therefore, account for the observed differences between the binding energies per nucleon. We can thus summarize this part of our discussion by stating that the discrepancy between experiment and theory observed in Table I can be ascribed to the missing three-body interactions, which are not included in our effective Hamiltonians. The advantage of the  $\text{N}^3\text{LO}$  model and similar models based on effective field theory, is that they allow for a consistent derivation of three-body terms (see, for example, Refs. [30, 123]). However, we have not developed the coupled-cluster codes for dealing with such interactions yet. We plan to do it in the future work.

It is interesting to observe that although the PR-EOMCCSD/CCSD/PA-EOMCCSD approaches underbind the five nuclei by about 1–1.4 MeV per particle, pointing to the need for the incorporation of three-body forces, the relative binding energies of  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{16}\text{O}$ ,  $^{17}\text{O}$ , and  $^{17}\text{F}$  obtained in coupled-cluster calculations are in good agreement with experiment. For exam-

ple, the difference between experimental binding energies of  $^{16}\text{O}$  and  $^{17}\text{O}$  is 0.225 MeV per particle. The CCSD and PA-EOMCCSD ground-state energies of  $^{16}\text{O}$  and  $^{17}\text{O}$  resulting from the calculations with eight major oscillator shells differ by 0.229 MeV per particle, in excellent agreement with experiment. The differences between the binding energies for the  $A = 15$  nuclei and for the  $A = 17$  nuclei are close to the experimental values too. From Table I, we extract  $\text{BE}(^{15}\text{N}) - \text{BE}(^{15}\text{O}) = 0.181$  MeV per particle, when the PR-EOMCCSD/ $\text{N}^3\text{LO}$  approach with eight major shells is employed, and 0.235 MeV per particle, when the experimental data are used ( $\text{BE} = \text{binding energy}$ ). Similarly, the PA-EOMCCSD/ $\text{N}^3\text{LO}$  calculations with eight major shells give  $\text{BE}(^{17}\text{O}) - \text{BE}(^{17}\text{F}) = 0.163$  MeV per particle, which is in reasonable agreement with the experimental result of 0.209 MeV per particle. The binding energies per nucleon resulting from the PR-EOMCCSD/CCSD/PA-EOMCCSD calculations satisfy the ordering  $^{15}\text{O} < ^{15}\text{N} < ^{17}\text{F} < ^{17}\text{O} < ^{16}\text{O}$ . With an exception of the  $^{15}\text{N}$  and  $^{17}\text{F}$  nuclei, whose binding energies per particle are close to each other and ordered in experiment as  $^{17}\text{F} < ^{15}\text{N}$ , the ordering resulting from the PR-EOMCCSD/CCSD/PA-EOMCCSD calculations is correct. This clearly illustrates that a great deal of useful information can be extracted from the relatively inexpensive coupled-cluster calculations of the CCSD type employing two-body interactions. The total binding energies are affected by three-body forces. However, the relative binding energies for the nuclei around  $^{16}\text{O}$  seem to be reasonably well described at the two-body interaction level when the coupled-cluster methods are used to describe particle correlations.

We end this subsection by tabulating the results of the PR-EOMCCSD and PA-EOMCCSD calculations for the low-lying excited states of  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$ , and  $^{17}\text{F}$  obtained with the  $\text{N}^3\text{LO}$  potential (see Table II; the experimental data are taken from Ref. [124]). Except for the  $(3/2)_1^+$  resonance states in  $^{17}\text{O}$  and  $^{17}\text{F}$ , all the other excited states listed in Table II are expected to be strongly dominated by one quasi-particle or quasi-hole states, meaning that the inclusion of the  $1p$  and  $2p-1h$  excitations in the PA-EOMCCSD calculations and the  $1h$  and  $2h-1p$  correlations in the PR-EOMCCSD calculations should provide a reasonable description of these states. This is confirmed in Table II. The PR-EOMCCSD/ $\text{N}^3\text{LO}$  results for the  $(3/2)_1^-$  states of  $^{15}\text{O}$  and  $^{15}\text{N}$ , employing seven or eight major oscillator shells, are particularly impressive, producing errors relative to experiment that do not exceed 0.1 MeV. For the particle case, the  $^{17}\text{O}$   $(1/2)_1^+$  excited state resulting from the PA-EOMCCSD calculations is slightly below the  $(5/2)_1^+$  ground state of  $^{17}\text{O}$ , when the  $\text{N}^3\text{LO}$  interaction and eight oscillator shells are employed. Else, the agreement with the experimental data is quite satisfactory. Again, as in Table I, we note a reasonably good convergence in the PR-EOMCCSD and PA-EOMCCSD results for the low-lying excited states of  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$ , and  $^{17}\text{F}$  in terms of

TABLE II: Energies of the low-lying excited states of  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$  and  $^{17}\text{F}$ , relative to the corresponding ground-state energies (the  $(1/2)_1^-$  states of  $^{15}\text{O}$  and  $^{15}\text{N}$  and the  $(5/2)_1^+$  states of  $^{17}\text{O}$  and  $^{17}\text{F}$ ), computed with the  $\text{N}^3\text{LO}$  interaction model [30] and the PR-EOMCCSD ( $^{15}\text{O}$ ,  $^{15}\text{N}$ ) and PA-EOMCCSD ( $^{17}\text{O}$  and  $^{17}\text{F}$ ) methods, as functions of the number of major oscillator shells  $N$ . All entries are in MeV. Note that the experimentally observed  $(3/2)_1^+$  states in  $^{17}\text{O}$  and  $^{17}\text{F}$  are resonances. The experimental data (Expt) are from Ref. [124]. For the optimum values of  $\hbar\Omega$  and  $\beta_{\text{COM}}$ , see Table I.

Excited state	$N = 5$	$N = 6$	$N = 7$	$N = 8$	Expt
$^{15}\text{O}$ $(3/2)_1^-$	6.515	6.602	6.166	6.264	6.176
$^{15}\text{N}$ $(3/2)_1^-$	6.354	6.680	6.256	6.318	6.323
$^{17}\text{O}$ $(3/2)_1^+$	6.298	6.031	5.489	5.675	5.084
$^{17}\text{O}$ $(1/2)_1^+$	0.328	0.130	-0.349	-0.025	0.870
$^{17}\text{F}$ $(3/2)_1^+$	6.460	6.207	5.686	5.891	5.000
$^{17}\text{F}$ $(1/2)_1^+$	0.748	0.544	0.088	0.428	0.495

the number of harmonic oscillator shells in a basis, which is yet another confirmation of the effectiveness of our computational procedure, in which we perform coupled-cluster calculations with the renormalized form of the Hamiltonian rather than with the underlying bare interactions that would lead to a very slow convergence rate with the number of single-particle states, making the calculations unmanageable.

Within a single-particle picture, the splitting between the  $(3/2)_1^-$  excited and  $(1/2)_1^-$  ground states in  $^{15}\text{O}$  and  $^{15}\text{N}$  and the splitting between the  $(3/2)_1^+$  excited and  $(5/2)_1^+$  ground states in  $^{17}\text{O}$  and  $^{17}\text{F}$  should arise from the nuclear spin-orbit force. It is interesting to analyze to what extent the three-nucleon interactions may affect these splittings. The nucleon-nucleon interaction contains a short-range spin-orbit force, which in a meson-exchange model picture originates from heavier vector mesons. Several partial waves receive significant contributions from the two-body spin-orbit force. For example, the  $^3P_2$  partial wave, crucial for the pairing properties in nuclei and neutron star matter, yields an attractive interaction up to almost 1 GeV in laboratory energy for the two-nucleon scattering. This attraction arises from the two-body spin-orbit force, since both the central and tensor force contributions are repulsive. Within the framework of many-body perturbation theory, the largest contribution to the spin-orbit force arises from the first-order Hartree-Fock diagram. Indeed, for the  $\text{N}^3\text{LO}$  model used here and for an oscillator energy  $\hbar\Omega = 14$  MeV, we obtain an excitation energy of 5.412 MeV for the  $0p_{3/2}$  state of  $^{15}\text{O}$ , in reasonable agreement with the experimental and coupled-cluster data in Table II [125]. At the Hartree-Fock diagram level, the origin of the spin-orbit splitting comes then from the renormalization of the short range two-body spin-orbit force. The nuclear tensor force gives also, as a second- and higher-order process, a contribu-

tion to the single-particle spin-orbit splitting (see the detailed discussion in Ref. [2] for further information). The authors of Ref. [2] show how the second-order diagrams in many-body perturbation theory with the  $2h$ - $1p$  and  $2p$ - $1h$  intermediate states yield repulsive and attractive contributions to the single-particle energies, respectively. Depending on the strength of the nuclear tensor force, the spin-orbit splittings can then be enhanced or reduced. If the tensor force is weak, as is the case for the  $N^3LO$  model, the reduced higher-order quenching of the tensor force terms enhances the spin-orbit splitting with respect to the Hartree-Fock diagram. Anticipating the discussion in Sec. III C, potentials with a stronger tensor force, such as the  $V_{18}$  model of the Argonne group [27], result in a smaller spin-orbit splitting than the  $N^3LO$  model (and a reduction in the  $(3/2)_1^- - (1/2)_1^-$  and  $(3/2)_1^+ - (5/2)_1^+$  spacings in the  $^{15}O/^{15}N$  and  $^{17}O/^{17}F$  nuclei, respectively). The authors of Refs. [1, 2] demonstrated then that a two-pion three-nucleon interaction also contributes to the spin-orbit splitting. With the inclusion of such a term, Pieper and Pandharipande [1], reproduced very well the  $(3/2)_1^- - (1/2)_1^-$  splitting in  $^{15}N$ . These findings were later corroborated by Heisenberg and Mihaila in their coupled-cluster calculations with three-body interactions for  $^{16}O$  (see Refs. [31, 32, 33, 34] and the discussion in the next subsection as well). The fact that we reproduce very well the experimental  $(3/2)_1^- - (1/2)_1^-$  spin-orbit splittings in  $^{15}N$  and  $^{15}O$  with the pairwise  $N^3LO$  model indicates that the spin-orbit force associated with an eventual three-body force for  $N^3LO$  should be small. This may be an important finding for our understanding of the role of three-body forces in nuclear structure calculations.

In Sec. III C, we present results for the binding energies and spectra of the  $^{15}N$  and  $^{15}O$  nuclei and their  $^{17}F$  and  $^{17}O$  counterparts using the CD-Bonn [28] and the Argonne  $V_{18}$  [27] interaction models as well, so that we can see how much the effects due to three-body interactions may depend on the underlying two-body forces. However, before we proceed, let us discuss interesting consequences of our PR-EOMCCSD and PA-EOMCCSD calculations for  $^{15}N$ ,  $^{15}O$ ,  $^{17}F$ , and  $^{17}O$  for the nuclear structure studies of the excited states of  $^{16}O$ .

### B. Consequences of the PR-EOMCCSD and PA-EOMCCSD Calculations for the Valence Systems around $^{16}O$ for the Studies of Excitations in $^{16}O$

Based on the  $N^3LO$  results discussed in the previous subsection, we attempt to link our findings to nuclear structure studies of the excitations in  $^{16}O$ . The fact that we obtain practically converged results for a given two-body Hamiltonian allows us to infer that eventual disagreements with experiment in the results of *ab initio* calculations for excited states of  $^{16}O$  can very likely be retraced to the degrees of freedom that are not included

in the existing two-body Hamiltonians.

Here, we discuss the excited states of  $^{16}O$  with an expected  $1p$ - $1h$  structure. In Ref. [37], we obtained converged results for the lowest-lying  $3_1^-$  state of  $^{16}O$ . For the  $N^3LO$  interaction, we obtained an excitation energy of about 12 MeV, almost 6 MeV above the experimental value of 6.13 MeV. The same Hamiltonian as that used here was employed. The low-lying excited states of  $^{16}O$  and, in general, states which involve cross-shell excitations, have always eluded a proper microscopic description (see, for example, Refs. [126, 127, 128, 129, 130, 131] and references therein).

Let us concentrate on the lowest-energy  $3_1^-$  state of  $^{16}O$ . In a zero-order approximation, this state may be regarded as a state that arises from the single  $i \rightarrow a$  excitation from the  $i = 0p_{1/2}$  hole state to the  $a = 0d_{5/2}$  particle state. Relative to the  $^{16}O$  ground state, the energy required to produce such an excitation equals

$$\begin{aligned} \Delta\epsilon_\pi &= \epsilon_\pi(0d_{5/2}) - \epsilon_\pi(0p_{1/2}) \\ &= [BE(^{16}O) - BE(^{17}F)] + [BE(^{16}O) - BE(^{15}N)] \\ &= 11.526 \text{ MeV}, \end{aligned} \quad (50)$$

for the proton case, and

$$\begin{aligned} \Delta\epsilon_\nu &= \epsilon_\nu(0d_{5/2}) - \epsilon_\nu(0p_{1/2}) \\ &= [BE(^{16}O) - BE(^{17}O)] + [BE(^{16}O) - BE(^{15}O)] \\ &= 11.521 \text{ MeV}, \end{aligned} \quad (51)$$

for the neutron case, where BE's in the above equations represent the relevant total binding energies. In calculating the above values of the  $1p$ - $1h$  excitation energies  $\Delta\epsilon_\pi$  and  $\Delta\epsilon_\nu$  that provide us with the zero-order estimates of the excitation energy of the lowest  $3_1^-$  state of  $^{16}O$ , we used the experimental binding energies listed in Table I. As we can see from Eqs. (50) and (51), the proton and neutron excitation energies are practically identical. This reflects a well-known feature of the spin-isospin saturated systems. Without interactions among nucleons and with the above single-particle orbits used as the only active degrees of freedom, all negative parity states with quantum numbers  $J^\pi = 2^-, 3^-$  would be at the above energies of approximately 11.5 MeV. The interactions among nucleons lower the energy of the first-excited  $3^-$  state by  $11.5 - 6.1 = 5.4$  MeV.

Let us now compare the approximate energy spacing defining the lowest  $3^-$  state of  $^{16}O$ , resulting from the use of experimental binding energies, as shown above (11.5 MeV), with the values of  $\Delta\epsilon_\pi$  and  $\Delta\epsilon_\nu$  based on the results of coupled-cluster calculations for the binding energies of  $^{16}O$  and valence systems around  $^{16}O$  obtained with the  $N^3LO$  interaction and eight major oscillator shells. These results are  $\Delta\epsilon_\pi = 15.846$  MeV and  $\Delta\epsilon_\nu = 15.789$  MeV, for proton and neutron excitations, respectively, with almost the same difference between the proton and neutron cases as observed in experiment. The authors of Ref. [115] obtained 14.72 MeV and 14.64 MeV for protons and neutrons, respectively, using the same

$N^3LO$  interaction as used here. We should note, however, that their results for  $^{16}O$  are not fully converged as a function of the model space size. Using the above elementary picture of the  $1p-1h$  excitation defining the lowest  $3^-$  state of  $^{16}O$ , which involves only two orbits in the definition of the relevant model space, we can see that we are off by approximately  $15.8 - 11.5 = 4.3$  MeV, when we compare the  $\Delta\epsilon_\pi$  and  $\Delta\epsilon_\nu$  energy spacings resulting from coupled-cluster calculations with the experimental estimates of these spacings. This difference is obviously an interaction and method dependent result. It is, however, converged as a function of the number of oscillator shells in a basis set, showing that the discrepancy of 4.3 MeV between theory and experiment for the energy gap between the  $0p$  and  $1s0d$  shells accounts for a large fraction of the missing 6 MeV needed to reproduce the first  $3^-$  state of  $^{16}O$ . This is, perhaps, the most likely candidate for a consistent explanation of the large difference between converged coupled-cluster result for the lowest  $3^-$  state of  $^{16}O$  and experiment reported in Ref. [37]. The above analysis indicates that a large fraction of the difference between theory and experiment can be traced in this case to errors in reproducing the experimental binding energies of  $^{16}O$  and valence systems around  $^{16}O$  by coupled-cluster methods employing pairwise interactions only. This allows us to conclude that a 6 MeV difference between coupled-cluster result and experiment for the lowest  $3^-$  state of  $^{16}O$  is primarily caused by the lack of three-body interactions in our calculations, and much less by the approximate treatment of particle correlations by the coupled-cluster methods used in our studies. The above analysis also implies that with an adjusted gap between the  $0p$  and  $1s0d$  shells, one should be able to get a better reproduction of the excited states of  $^{16}O$  which have a well-defined  $1p-1h$  structure, such as the lowest  $3^-$  state discussed here. One possible strategy for describing excited states of closed-shell nuclei dominated by  $1p-1h$  excitations might be to keep the original two-body Hamiltonian and add additional three-body terms via corrections to the single-particle energies, as advocated recently by Zuker [132, 133].

### C. Results for Other Interaction Models

The binding energies per particle for the three interaction models examined in this work, namely  $N^3LO$ , CD-Bonn, and  $V_{18}$ , are listed in Table III. We only show the essentially converged results obtained with eight major oscillator shells, since convergence patterns with the number of major oscillator shells that characterize the  $N^3LO$ , CD-Bonn, and  $V_{18}$  interactions are practically identical.

As expected, the CD-Bonn interaction gives more attraction than  $N^3LO$ , while the Argonne  $V_{18}$  interaction model yields less attraction than the other two models. The CD-Bonn potential has the weakest tensor force of the three interactions studied here, whereas the  $V_{18}$  in-

teraction has the strongest tensor force component. It is well-known that an interaction model with a weak tensor force yields less quenching in the medium for the important  $^3S_1$  and  $^3D_1$  partial wave contributions to various matrix elements of the Hamiltonian. The quenching is ascribed to both a Pauli effect and an energy dependence reflected in second- and higher-order terms (see, for example, Ref. [5] for a discussion of this topic in both nuclei and nuclear matter). Although all interaction models fit properties of the deuteron and the scattering data with a  $\chi^2$  per datum close to 1, the non-localities which are introduced due to the way the interactions are constructed are responsible for different results in a many-body context. Indeed, the  $N^3LO$  and CD-Bonn models are non-

TABLE III: A comparison of the binding energies per particle for  $^{15}O$  and  $^{15}N$  (the PR-EOMCCSD values),  $^{16}O$  (the CCSD values), and  $^{17}O$  and  $^{17}F$  (the PA-EOMCCSD values), obtained with the  $N^3LO$  [30], CD-Bonn [28], and  $V_{18}$  [27] potentials, and eight major oscillator shells, with the experimental data taken from Ref. [120]. All entries are in MeV. For the CD-Bonn and  $N^3LO$  interactions, we used  $\hbar\Omega = 11$  MeV. For  $V_{18}$ , we used  $\hbar\Omega = 10$  MeV. For eight major shells, the results are practically independent of the choice of  $\hbar\Omega$  and  $\beta_{\text{COM}} = 0.0$ .

Nucleus	Interaction			Expt
	$N^3LO$	CD-Bonn	$V_{18}$	
$^{15}O$	6.158	6.643	4.789	7.464
$^{15}N$	6.339	6.810	4.957	7.699
$^{16}O$	6.951	7.444	5.469	7.976
$^{17}O$	6.722	7.201	5.214	7.751
$^{17}F$	6.559	7.048	5.059	7.542

local interactions defined in momentum space. While the  $N^3LO$  model is based on chiral Lagrangians with nucleons and pions as degrees of freedom, including the non-iterative  $2\pi$  diagrams at chiral fourth order, the CD-Bonn interaction is a traditional meson-exchange model that includes the six low-mass mesons  $\pi, \delta, \rho, \omega, \eta$  and the fictitious  $\sigma$  meson, which is a  $2\pi$  resonance. The Argonne  $V_{18}$  model is based on a local  $r$ -space parametrization, dominated by one-pion exchange. The strength of the nuclear tensor force is intimately connected with the non-localities of the different nucleon-nucleon forces. Depending on how it is quenched in a many-body context, one may get less or more attraction. The attractive part of, for example, the  $^3S_1$  partial wave contribution is more attractive in the medium for an interaction with a weak tensor than for one with a strong tensor force. Such features are clearly seen in the coupled-cluster results reported in Table III, where the potential with the weakest tensor force, CD-Bonn, yields more binding than the two other models.

As mentioned previously, our results are practically converged as functions of the number of harmonic oscillator shells. Based on our earlier work [37], the triply



excited clusters and the related  $3p-2h$  and  $3h-2p$  excitations in the particle-attaching and particle-removing  $R_\mu^{(A+1)}$  and  $R_\mu^{(A-1)}$  operators of the PA-EOMCC and PR-EOMCC theories are expected to have very little impact on the calculated binding energies. We claim therefore that, except for a small correction due to triples and a weak starting energy dependence [37], the lack of agreement between coupled-cluster and experimental binding energies is primarily due to the missing physics in our Hamiltonians. The main conclusion that one can derive from the results of our coupled-cluster calculations with different interactions is that every nucleon-nucleon interaction model needs its own three-body potential. The Argonne group has derived sophisticated three-body interaction terms (see, for example, the extensive elaboration of Ref. [134]). The parameters entering their three-body interaction models are fitted to reproduce properties of light nuclei. These three-body terms follow much of the same pion-exchange picture adopted in the construction of the Argonne  $V_{18}$  interaction. For the CD-Bonn interaction one would need to derive three-body terms based on a meson-exchange picture, as outlined, for example, by the Bochum group [135]. However, no such model, which accompanies this interaction, has been fully developed. The situation for models based on effective field theory is much better as three-body terms arise quite naturally at given orders in the expansion parameter [123]. Our coupled-cluster results indicate that every interaction, due to different non-localities, has its own three-body component reflected in different binding energies and different spin-orbit splittings (the  $(3/2)_1^- - (1/2)_1^-$  spacings in  $^{15}\text{O}$  and  $^{15}\text{N}$  and the  $(3/2)_1^+ - (5/2)_1^+$  spacings in  $^{17}\text{O}$  and  $^{17}\text{F}$ ), as demonstrated in Table III, which lists binding energies per nucleon, and Table IV, which lists the corresponding low-lying excited states of the valence systems around  $^{16}\text{O}$  examined in this work.

As shown in Table IV, the CD-Bonn and the  $\text{N}^3\text{LO}$  models result in the largest spin-orbit splittings (much larger than in the case of  $V_{18}$ ). In order to examine this behavior in some detail, we have computed all diagrams through third order in the  $G$  matrix for  $\hbar\Omega = 14$  MeV, using many-body perturbation theory as described in Ref. [5], including folded diagrams to infinite order. For example, at the Hartree-Fock level, which corresponds to the first order in the  $G$  matrix, the spin-orbit splittings for neutrons between the two hole states in the  $0p$  shell are 4.85 MeV, 4.41 MeV, and 3.91 MeV for the CD-Bonn,  $\text{N}^3\text{LO}$  and  $V_{18}$  interaction models, respectively. Since we are dealing with spin-isospin saturated systems, the results for protons are almost the same. The Hartree-Fock term yields the largest contribution and receives important contributions from the short-range two-body spin-orbit force. However, there is also a considerable contribution to the splitting that originates from the second-order  $2h-1p$  and  $2p-1h$  terms. The corresponding second-order contributions are 1.81 MeV, 1.73 MeV and 1.35 MeV for the same three interactions, respectively. These perturbation theory estimates agree with

TABLE IV: A comparison of the energies of the low-lying excited states of  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$  and  $^{17}\text{F}$ , relative to the corresponding ground-state energies (the  $(1/2)_1^-$  states of  $^{15}\text{O}$  and  $^{15}\text{N}$  and the  $(5/2)_1^+$  states of  $^{17}\text{O}$  and  $^{17}\text{F}$ ), obtained with the PR-EOMCCSD ( $^{15}\text{O}$  and  $^{15}\text{N}$ ) and PA-EOMCCSD ( $^{17}\text{O}$  and  $^{17}\text{F}$ ) methods, the  $\text{N}^3\text{LO}$  [30], CD-Bonn [28], and  $V_{18}$  [27] potentials, and eight major oscillator shells, with the experimental data taken from Ref. [124]. All entries are in MeV. For the CD-Bonn and  $\text{N}^3\text{LO}$  interactions, we used  $\hbar\Omega = 11$  MeV. For  $V_{18}$ , we used  $\hbar\Omega = 10$  MeV. For eight major shells, the results are practically independent of the choice of  $\hbar\Omega$  and  $\beta_{\text{CoM}} = 0.0$ .

Excited state	Interaction			Expt
	$\text{N}^3\text{LO}$	CD-Bonn	$V_{18}$	
$^{15}\text{O} (3/2)_1^-$	6.264	7.351	4.452	6.176
$^{15}\text{N} (3/2)_1^-$	6.318	7.443	4.499	6.323
$^{17}\text{O} (3/2)_1^+$	5.675	6.406	3.946	5.084
$^{17}\text{O} (1/2)_1^+$	-0.025	0.311	-0.390	0.870
$^{17}\text{F} (3/2)_1^+$	5.891	6.677	4.163	5.000
$^{17}\text{F} (1/2)_1^+$	0.428	0.805	0.062	0.495

the ways the  $(3/2)_1^- - (1/2)_1^-$  spacings in  $^{15}\text{O}$  and  $^{15}\text{N}$  and the  $(3/2)_1^+ - (5/2)_1^+$  spacings in  $^{17}\text{O}$  and  $^{17}\text{F}$ , obtained in the corresponding PR-EOMCCSD and PA-EOMCCSD calculations, vary with the interaction. This analysis illustrates, at least to some extent, the role played by the quenching of the tensor force via the second and higher-order terms in many-body perturbation theory in different interaction models. The perturbative results do not stabilize, however, as functions of the oscillator energy, a result which is in close agreement with the findings reported by Fujii *et al.* [115]. With increasing  $\hbar\Omega$ , the single-particle splittings increase if one uses an unperturbed harmonic oscillator basis. We defer thus from a more elaborate analysis of many-body perturbation theory, since it yields results of a rather limited interest. The problems with many-body perturbation theory, such as the lack of a proper indication of convergence in terms of  $G$  and the difficulties with going beyond third order in the interaction, are well known. The coupled-cluster methods, including the quantum chemistry inspired CCSD, PA-EOMCCSD, and PR-EOMCCSD approximations used in this work, are capable of summing large classes of diagrams to infinite order, eliminating many of the problems encountered in many-body perturbation theory calculations, and providing a much more stable description of the ground and excited states of the valence systems around  $^{16}\text{O}$ . The differences between coupled-cluster results obtained with different interactions point to the need for developing three-body interactions consistent with a given two-body interaction model.

It is interesting to note that in spite of the apparent differences between the converged coupled-cluster results obtained with different pairwise interaction models, the relative binding energies of  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{16}\text{O}$ ,  $^{17}\text{O}$ , and  $^{17}\text{F}$

obtained with different interactions are in good agreement with experiment and with each other. For example, as already mentioned the difference between experimental binding energies of  $^{16}\text{O}$  and  $^{17}\text{O}$  is 0.225 MeV per particle. The CCSD and PA-EOMCCSD ground-state energies of  $^{16}\text{O}$  and  $^{17}\text{O}$  resulting from the calculations with eight major oscillator shells differ by 0.229 MeV per particle for  $\text{N}^3\text{LO}$ , 0.243 MeV per particle for CD-Bonn, and 0.255 MeV per particle for  $V_{18}$ . Similarly, the difference between experimental binding energies of  $^{16}\text{O}$  and  $^{15}\text{O}$  is 0.512 MeV per particle, whereas the CCSD and PR-EOMCCSD ground-state energies of  $^{16}\text{O}$  and  $^{15}\text{O}$  differ by 0.793, 0.801, and 0.680 MeV per particle for the  $\text{N}^3\text{LO}$ , CD-Bonn, and  $V_{18}$  potentials, respectively. Here, the differences with experiment are somewhat greater than in the case of  $^{16}\text{O}$  and  $^{17}\text{O}$ , but the overall agreement among different potentials is still very good. The differences between the binding energies for the  $A = 15$  nuclei and for the  $A = 17$  nuclei obtained with different interactions are close to one another and to the experimental values too. According to Table III, the experimental value of the binding energy difference  $\text{BE}(^{15}\text{N}) - \text{BE}(^{15}\text{O})$  is 0.235 MeV per particle. The PR-EOMCCSD calculations with the  $\text{N}^3\text{LO}$ , CD-Bonn, and  $V_{18}$  interactions give 0.181, 0.167, and 0.168 MeV per particle, respectively, for the same binding energy difference. Similarly, the experimental value of the binding energy difference  $\text{BE}(^{17}\text{O}) - \text{BE}(^{17}\text{F})$  is 0.209 MeV per particle. The PA-EOMCCSD calculations with the  $\text{N}^3\text{LO}$ , CD-Bonn, and  $V_{18}$  potentials give 0.163, 0.153, and 0.155 MeV per particle, respectively, for the same binding energy difference. In spite of the substantial differences between binding energies resulting from the calculations with different interactions, which are affected by the three-body forces that are expected to be different for different pairwise interactions, the binding energies per nucleon resulting from our PR-EOMCCSD/CCSD/PA-EOMCCSD calculations with eight major oscillator shells satisfy  $^{15}\text{O} < ^{15}\text{N} < ^{17}\text{F} < ^{17}\text{O} < ^{16}\text{O}$ , independent of the interaction used in coupled-cluster calculations. This means that once we adjust the value of the binding energy of the reference  $^{16}\text{O}$  system, we can obtain the interaction-independent ordering of the binding energies of the valence nuclei around  $^{16}\text{O}$ . With an exception of the  $^{15}\text{N}$  and  $^{17}\text{F}$  nuclei, whose binding energy ordering should be reversed, the ordering of binding energies per particle resulting from the relatively inexpensive coupled-cluster calculations is in good agreement with experiment. These are encouraging findings from the point of view of the future applications of coupled-cluster methods employing renormalized Hamiltonians in nuclear physics.

#### IV. CONCLUSIONS AND PERSPECTIVES

We summarize here our main conclusions and perspectives for future studies.

1. To our knowledge, this is the first application of the *ab initio* coupled-cluster theory employing the renormalized form of the Hamiltonian, combined with the PA-EOMCC and PR-EOMCC formalisms for open-shell many-fermion systems, to nuclear valence systems with one valence particle or one valence hole. We have shown that one can obtain virtually converged results with given two-body Hamiltonians for both binding energies and low-lying excited states. This has been possible thanks to the development of highly efficient CCSD, PA-EOMCCSD, and PR-EOMCCSD computer codes and the use of the renormalized Hamiltonians in our calculations, which lead to a rapid convergence with the number of oscillator shells in a basis. The systems whose properties have been studied in this work were  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$  and  $^{17}\text{F}$ . An emphasis has been placed on states dominated by one-quasi-particle configurations. The discrepancies between the results of large-scale coupled-cluster calculations for these nuclei and the corresponding experimental data have been traced to the Hamiltonians used in the calculations, much less to the correlations neglected in coupled-cluster approximations employed in this study.
2. Three different nucleon-nucleon interactions have been used to define our two-body Hamiltonians. These are the  $\text{N}^3\text{LO}$  model [30], the CD-Bonn interaction [28], and the  $V_{18}$  model of the Argonne group [27]. All of these interactions yield different binding energies and different energies of the excited states. The different binding energies and spin-orbit splittings can be related to varying non-localities in the nucleon-nucleon interactions. Of particular interest here has been the role played by the nuclear tensor force. The different behavior of the three interaction models examined in this study points to the need for the development of the interaction specific three-body forces.
3. We have also demonstrated that most of the discrepancy between theory and experiment for the  $1p\text{-}1h$  negative parity states in  $^{16}\text{O}$ , including the lowest  $3_1^-$  state examined in our earlier work [37], can be retraced to the difference between the theoretical and experimental values of the relevant energy gaps between neutron or proton states in the  $0p$  and  $1s0d$  shells.
4. In spite of the differences among interactions, the relative binding energies of the  $^{15}\text{O}$ ,  $^{15}\text{N}$ ,  $^{17}\text{F}$ ,  $^{17}\text{O}$ , and  $^{16}\text{O}$  resulting from the coupled-cluster calculations seem to be virtually independent of the interaction and in good agreement with experiment. The  $(3/2)_1^- - (1/2)_1^-$  spacings in  $^{15}\text{O}$  and  $^{15}\text{N}$  resulting from the converged coupled-cluster calculations with the  $\text{N}^3\text{LO}$  interaction are in excellent agreement with experiment, indicating that the spin-

orbit force associated with an eventual three-body force for  $N^3LO$  should be small.

There are several obvious extensions to this work. First of all, the need for an inclusion of three-body interactions sets the agenda for forthcoming studies. Moreover, it may be useful to examine the role of  $3p-2h$  and  $3h-2p$  correlations in the PA-EOMCC and PR-EOMCC calculations, which we neglected in this study. For the states considered here, the  $3p-2h$  and  $3h-2p$  correlations are expected to be small, since the states of  $^{15}O$ ,  $^{15}N$ ,  $^{17}F$ , and  $^{17}O$  that we have examined show relatively small departures from an independent-particle picture and since the underlying  $T_3$  cluster contributions that define the reference  $^{16}O$  system are small [37]. On the other hand, we have tacitly assumed that the  $0d_{3/2}$  states of  $^{17}F$  and  $^{17}O$  are bound states. These states are resonances, and it is not yet entirely clear how the non-resonant continuum may affect the description of these states. The inclusion of such contributions in the description of these states is another important point to explore, as demonstrated in the recent works on the Gamow shell-model and complex-scaling techniques [136, 137, 138].

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### APPENDIX: FACTORIZED FORM OF THE CCSD, PA-EOMCCSD, AND PR-EOMCCSD EQUATIONS

In this appendix, we present the working equations defining the CCSD, PA-EOMCCSD, and PR-EOMCCSD

methods exploited in this study. All of the equations are expressed in terms of the one- and two-body matrix elements of the Hamiltonian in the normal-ordered form,  $f_\alpha^\beta$  and  $v_{\alpha\beta}^{\gamma\delta}$ , respectively (cf. Eq. (11); in our case,  $f_\alpha^\beta$  and  $v_{\alpha\beta}^{\gamma\delta}$  are the one- and two-body matrix elements of the normal-ordered form of the effective Hamiltonian  $\bar{H}$ , Eq. (2)), the  $t_a^i$  and  $t_{ab}^{ij}$  cluster amplitudes defining the underlying  $A$ -particle ground-state CCSD problem, and, in the case of the PA-EOMCCSD and PR-EOMCCSD approaches, the  $r_a$ ,  $r_{ab}^j$ ,  $r^i$ , and  $r_b^{ij}$  amplitudes defining the particle-attaching ( $r_a$  and  $r_{ab}^j$ ) and particle-removing ( $r^i$  and  $r_b^{ij}$ ) operators,  $R_\mu^{(A+1)}(2p-1h)$  and  $R_\mu^{(A-1)}(2h-1p)$ , Eqs. (33) and (34), respectively. As explained in Sec. II C, the CCSD, PA-EOMCCSD, and PR-EOMCCSD equations can be cast into a computationally efficient factorized form expressed in terms of the one- and two-body matrix elements of the CCSD similarity-transformed Hamiltonian  $\bar{H}_{N,\text{open}}(\text{CCSD})$ ,  $\bar{h}_\alpha^\beta$  and  $\bar{h}_{\alpha\beta}^{\gamma\delta}$ , respectively, and a few additional intermediates that are generated in a recursive manner. The complete set of one- and two-body matrix elements of  $\bar{H}_{N,\text{open}}(\text{CCSD})$  and other intermediates that are needed to set up the CCSD, PA-EOMCCSD, and PR-EOMCCSD equations is given in Table V.

The ground-state CCSD equations for the singly and doubly excited cluster amplitudes  $t_a^i$  and  $t_{ab}^{ij}$ , Eqs. (21) and (22), can be given the following, computationally efficient form:

$$\begin{aligned} \bar{h}_a^i \equiv & f_a^i + I_a^e t_e^i - \bar{h}_m^i t_a^m - v_{ma}^{ie} t_e^m + \bar{h}_m^e t_{ea}^{mi} - \frac{1}{2} \bar{h}_{mn}^{ie} t_{ae}^{mn} \\ & + \frac{1}{2} v_{am}^{ef} t_{ef}^{im} = 0, \end{aligned} \quad (\text{A.1})$$

$$\begin{aligned} \bar{h}_{ab}^{ij} \equiv & v_{ab}^{ij} + \mathcal{A}_{ab} \mathcal{A}^{ij} [\frac{1}{2} I_{ab}^{ie} t_e^{ij} - \frac{1}{2} I_{mb}^{ij} t_a^m + \frac{1}{2} I_b^{e,ij} t_{ae}^{ie} \\ & + \frac{1}{8} v_{ab}^{ef} t_{ef}^{ij} + \frac{1}{8} \bar{h}_{mn}^{ij} t_{ab}^{mn} - I_{mb}^{ie} t_{ae}^{mj} - \frac{1}{2} \bar{h}_m^{ij} t_{ab}^{im}] \\ = & 0. \end{aligned} \quad (\text{A.2})$$

Note that the left-hand sides of Eqs. (21) and (22) (or (A.1) and (A.2)) represent, respectively, the one- and two-body matrix elements  $\bar{h}_a^i$  and  $\bar{h}_{ab}^{ij}$  of  $\bar{H}_N(\text{CCSD})$  (see Eqs. (12) and (13)). The relevant intermediates can be found in Table V. The antisymmetrizers  $\mathcal{A}_{pq} = \mathcal{A}^{pq}$ , which enter Eq. (A.2) and other equations presented in this appendix, are defined as

$$\mathcal{A}_{pq} \equiv \mathcal{A}^{pq} = 1 - (pq), \quad (\text{A.3})$$

with  $(pq)$  representing a transposition of two indices. Once the above equations are solved for  $t_a^i$  and  $t_{ab}^{ij}$ , the ground-state CCSD energy is calculated using the formula (cf. Eq. (20))

$$E_0^{(A)}(M) = \langle \Phi | H | \Phi \rangle + f_a^a t_a^a + \frac{1}{4} v_{ij}^{ab} (t_{ab}^{ij} + 2 t_a^i t_b^j), \quad (\text{A.4})$$

which is valid for any truncation scheme  $M \geq 2$ .

Once the  $t_a^i$  and  $t_{ab}^{ij}$  amplitudes are determined and the ground-state CCSD energy of the reference  $A$ -body

TABLE V: Explicit algebraic expressions for the one- and two-body matrix elements elements of  $\bar{H}_{N,\text{open}}(\text{CCSD})$  ( $\bar{h}_\alpha^\beta$  and  $\bar{h}_{\alpha\beta}^{\gamma\delta}$ , respectively) and other intermediates (designated by  $I$ ) used to construct the computationally efficient form of the CCSD, PA-EOMCCSD, and PR-EOMCCSD equations.

Intermediate	Expression <sup>a</sup>
$\bar{h}_i^a$	$f_i^a + v_{im}^{ae} t_e^m$
$\bar{h}_i^j$	$f_i^j + v_{im}^{je} t_e^m + \frac{1}{2} v_{mi}^{ef} t_{ef}^{mj} + \bar{h}_i^e t_e^j$
$\bar{h}_a^b$	$I_a^b - \bar{h}_m^b t_a^m$
$\bar{h}_{ai}^{bc}$	$v_{ai}^{bc} - v_{mi}^{bc} t_a^m$
$\bar{h}_{ij}^{ka}$	$v_{ij}^{ka} + v_{ia}^{ea} t_e^k$
$\bar{h}_{ab}^{cd}$	$v_{ab}^{cd} + \frac{1}{2} v_{mn}^{cd} t_{ab}^{mn} - \bar{h}_{am}^{cd} t_b^m + v_{bm}^{cd} t_a^m$
$\bar{h}_{ij}^{kl}$	$v_{ij}^{kl} + \frac{1}{2} v_{ij}^{ef} t_{ef}^{kl} - \bar{h}_{ij}^{le} t_e^k + v_{ij}^{ke} t_e^l$
$\bar{h}_{ia}^{jb}$	$I_{ia}^{jb} - v_{im}^{eb} t_{ea}^{jm} - \bar{h}_{im}^{jb} t_a^m$
$\bar{h}_{ab}^{ic}$	$v_{ab}^{ic} + v_{ab}^{ec} t_e^i - \bar{h}_{mb}^{ic} t_a^m + I_{ma}^{ic} t_b^m$ $- \bar{h}_m^{ic} t_{ab}^{im} + \bar{h}_{bm}^{ce} t_{ae}^{im} - v_{am}^{ce} t_{be}^{im} + \frac{1}{2} \bar{h}_{nm}^{ic} t_{ab}^{nm}$
$\bar{h}_{ia}^{jk}$	$v_{ia}^{jk} + \bar{h}_{mi}^{jk} t_a^m - v_{ia}^{ke} t_e^j + \mathcal{A}^{jk} \bar{h}_{im}^{je} t_{ae}^{km}$ $+ \bar{h}_i^{je} t_{ea}^{jk} + I_{ia}^{je} t_e^k - \frac{1}{2} v_{ai}^{ef} t_{ef}^{jk}$
$I_a^{fb}$	$f_a^b + v_{am}^{be} t_e^m$
$I_a^b$	$I_a^b - \frac{1}{2} v_{mn}^{eb} t_{ea}^{mn}$
$I_{ab}^{ic}$	$v_{ab}^{ic} + v_{ab}^{ec} t_e^i + v_{mb}^{ec} t_{ae}^{im}$
$I_{ia}^{jk}$	$\bar{h}_{ia}^{jk} - \frac{1}{2} \bar{h}_{mi}^{jk} t_a^m$
$I_{ia}^{jb}$	$-\frac{1}{2} v_{im}^{eb} t_{ea}^{jm}$
$I_{ia}^{jb}$	$v_{ia}^{jb} + v_{ia}^{eb} t_e^j$
$I_m$	$\frac{1}{2} v_{mn}^{ef} r_{ef}^n$
$I^e$	$-\frac{1}{2} v_{mn}^{ef} r_{ef}^{mn}$

<sup>a</sup>Summation over repeated upper and lower indices is assumed.  $f_\alpha^\beta = \langle \alpha | f | \beta \rangle$  and  $v_{\alpha\beta}^{\gamma\delta} = \langle \alpha\beta | v | \gamma\delta \rangle - \langle \alpha\beta | v | \delta\gamma \rangle$  are the one- and two-body matrix elements of the Hamiltonian in the normal-ordered form, Eq. (11) and the  $t_a^i$  and  $t_{ab}^{ij}$  are the singly and doubly excited cluster amplitudes defining the ground-state CCSD wave function of the  $A$ -body reference system.

system is known, we can set up and solve the eigenvalue equations defining the PA-EOMCCSD and PR-EOMCCSD methods. The PA-EOMCCSD equations for the energy differences  $\omega_\mu^{(A+1)} = E_\mu^{(A+1)} - E_0^{(A)}$  and the  $1p$  and  $2p\text{-}1h$  amplitudes,  $r_a$  and  $r_{ab}^j$ , respectively, defining the ground and excited states of the  $(A+1)$ -particle system, can be given the following, computationally efficient, form:

$$\langle \Phi^a | [\bar{H}_{N,\text{open}}(\text{CCSD}) R_\mu^{(A+1)}(2p\text{-}1h)]_C | \Phi \rangle = \bar{h}_a^e r_e + \bar{h}_m^e r_{ae}^m + \frac{1}{2} \bar{h}_{am}^{ef} r_{ef}^m = \omega_\mu^{(A+1)} r_a, \quad (\text{A.5})$$

$$\begin{aligned} \langle \Phi^{ab} | [\bar{H}_{N,\text{open}}(\text{CCSD}) R_\mu^{(A+1)}(2p\text{-}1h)]_C | \Phi \rangle &= \mathcal{A}_{ab} \left[ -\frac{1}{2} \bar{h}_{ab}^{je} r_e + \bar{h}_a^e r_{eb}^j - \frac{1}{2} \bar{h}_m^j r_{ab}^m + \frac{1}{4} \bar{h}_{ab}^{ef} r_{ef}^j - \bar{h}_{ma}^{je} r_{eb}^m - \frac{1}{2} I_m t_{ab}^{mj} \right] \\ &= \omega_\mu^{(A+1)} r_{ab}^j. \end{aligned} \quad (\text{A.6})$$

Similarly, we can use the CCSD values of the singly and doubly excited cluster amplitudes defining the ground-state wave function of the reference  $A$ -body system to set up the PR-EOMCCSD eigenvalue equations for the energy differences  $\omega_\mu^{(A-1)} = E_\mu^{(A-1)} - E_0^{(A)}$  and the  $1h$

and  $2h\text{-}1p$  amplitudes,  $r^i$  and  $r_b^{ij}$ , respectively, defining the ground and excited states of the  $(A-1)$ -particle system. The computationally efficient form of the PR-EOMCCSD equations is as follows:

$$\langle \Phi_i | [\bar{H}_{N,\text{open}}(\text{CCSD}) R_\mu^{(A-1)}(2h\text{-}1p)]_C | \Phi \rangle = -\bar{h}_m^i r^m + \bar{h}_m^e r_{e}^{im} - \frac{1}{2} \bar{h}_{mn}^{ie} r_e^{mn} = \omega_\mu^{(A-1)} r^i, \quad (\text{A.7})$$

$$\begin{aligned}
\langle \Phi_{ij}^b | [\bar{H}_{N,\text{open}}(\text{CCSD}) R_\mu^{(A-1)}(2h-1p)]_C | \Phi \rangle &= \mathcal{A}^{ij} \left[ -\frac{1}{2} \bar{h}_{mb}^{ij} r^m - \bar{h}_m^i r_b^{mj} + \frac{1}{2} \bar{h}_b^e r_e^{ij} + \frac{1}{4} \bar{h}_{mn}^{ij} r_b^{mn} - \bar{h}_{mb}^{ie} r_e^{mj} + \frac{1}{2} I^e t_{eb}^{ij} \right] \\
&= \omega_\mu^{(A-1)} r_b^{ij},
\end{aligned} \tag{A.8}$$

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